Full wwPDB EM Validation Report ⓘ

Apr 10, 2024 – 04:22 pm BST

PDB ID	:	8CRO
EMDB ID	:	EMD-16809
Title	:	Cryo-EM structure of Pyrococcus furiosus transcription elongation complex
Authors	:	Tarau, D.M.; Grunberger, F.; Reichelt, R.; Heiss, F.B.; Pilsl, M.; Hausner, W.; Engel, C.; Grohmann, D.
Deposited on	:	2023-03-08
Resolution	:	3.10 Å(reported)
Based on initial model	:	.

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

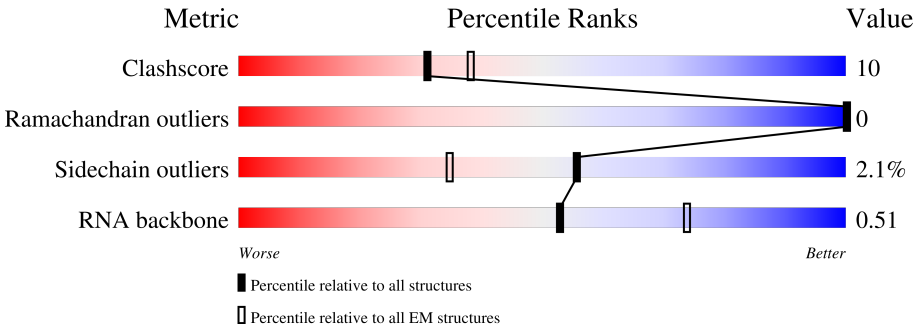
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	910	73% 25%
2	B	1117	75% 23%
3	C	397	12% 73% 24%
4	D	261	79% 20%
5	E	189	52% 71% 29%
6	F	120	28% 62% 34%
7	L	95	74% 25%

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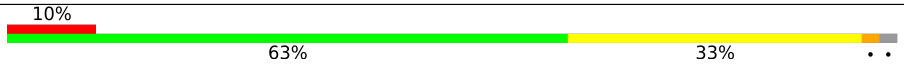
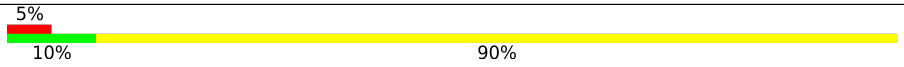
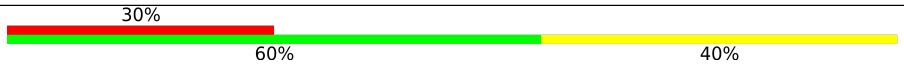
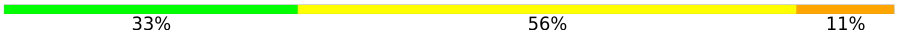
Mol	Chain	Length	Quality of chain
8	H	82	
9	N	65	
10	K	57	
11	P	49	
12	X	20	
13	Y	10	
14	Z	9	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 27169 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit Rpo1N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	900	7189	4536	1281	1334	38	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1098	8802	5578	1564	1626	34	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit Rpo1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	390	3057	1931	528	588	10	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit Rpo3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	258	2086	1358	330	396	2	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit Rpo7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	189	1528	990	253	279	6	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit Rpo4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	116	946	602	156	182	6	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit Rpo11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	94	Total	C	N	O	S	0	0
			777	500	129	146	2		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit Rpo5.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	76	Total	C	N	O	0	0
			609	398	100	111		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit Rpo10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	65	Total	C	N	O	S	0	0
			543	345	94	97	7		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit Rpo6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	55	Total	C	N	O	S	0	0
			424	281	71	71	1		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit Rpo12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	48	Total	C	N	O	S	0	0
			393	251	75	63	4		

- Molecule 12 is a DNA chain called DNA Template Strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	20	Total	C	N	O	P	0	0
			414	196	77	121	20		

- Molecule 13 is a DNA chain called DNA Non-Template Strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	10	Total	C	N	O	P	0	0
			199	96	33	60	10		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	9	Total	C	N	O	P	0	0
			196	87	39	61	9		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	A	2	Total	Zn	0
			2	2	
15	B	1	Total	Zn	0
			1	1	
15	N	1	Total	Zn	0
			1	1	
15	P	1	Total	Zn	0
			1	1	

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

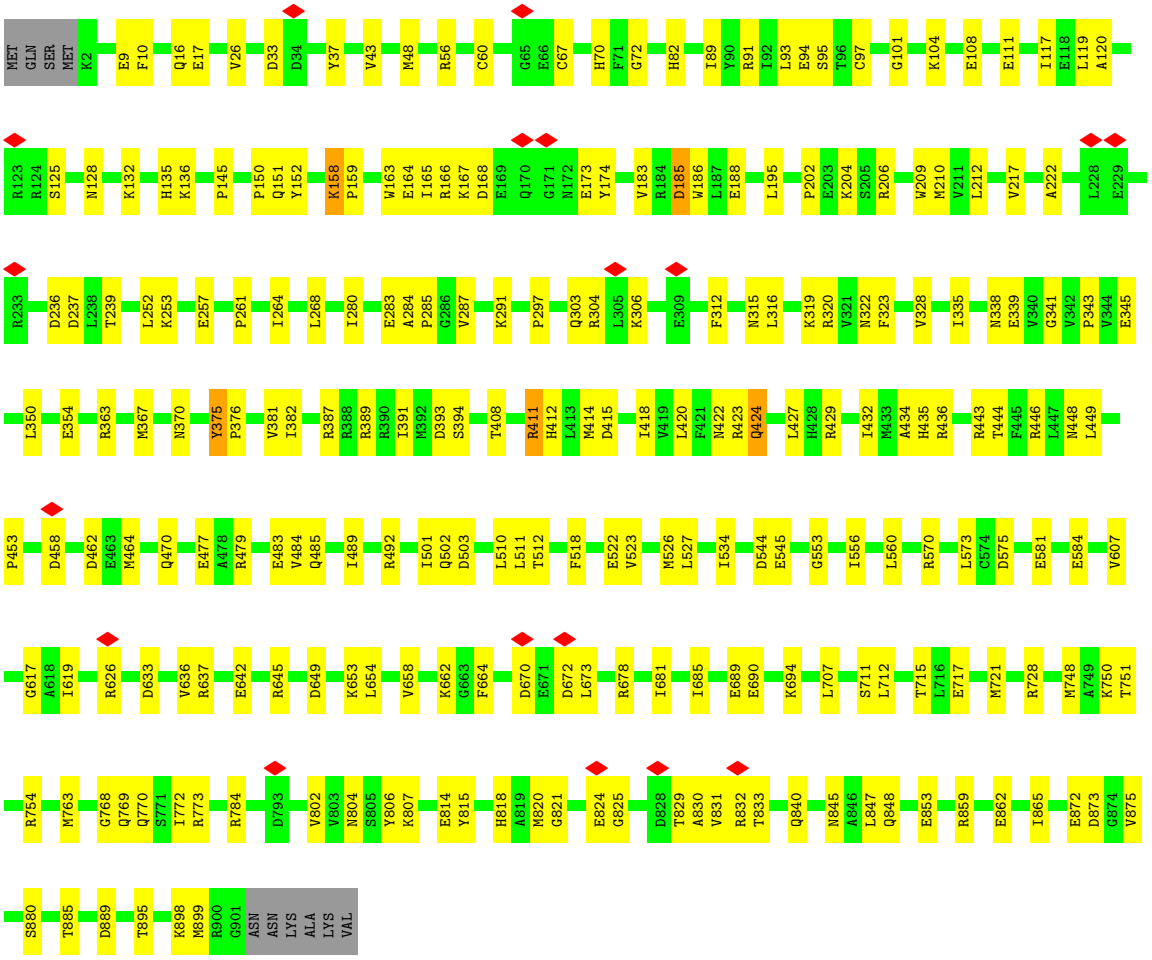
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

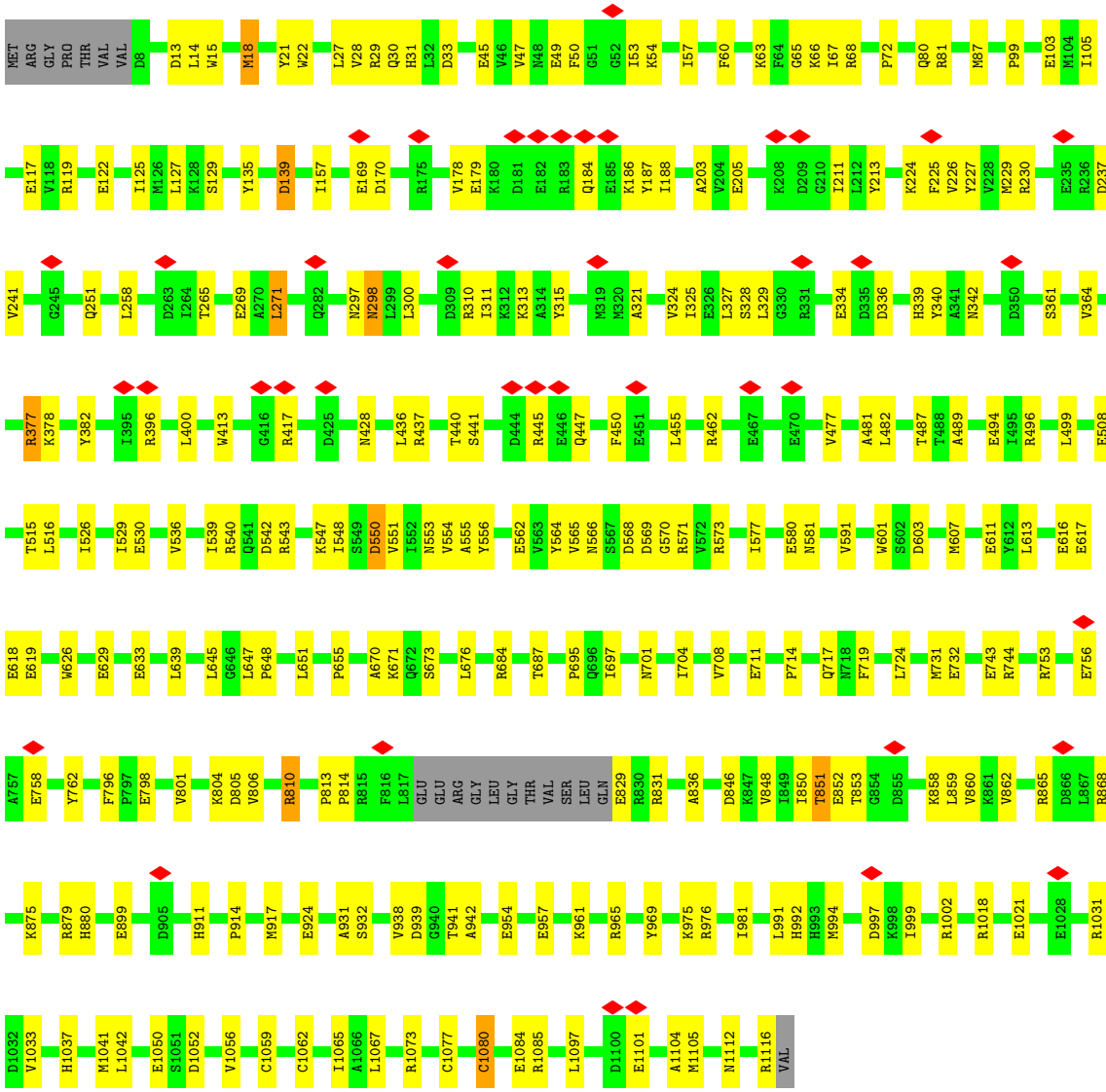
• Molecule 1: DNA-directed RNA polymerase subunit Rpo1N

Chain A:



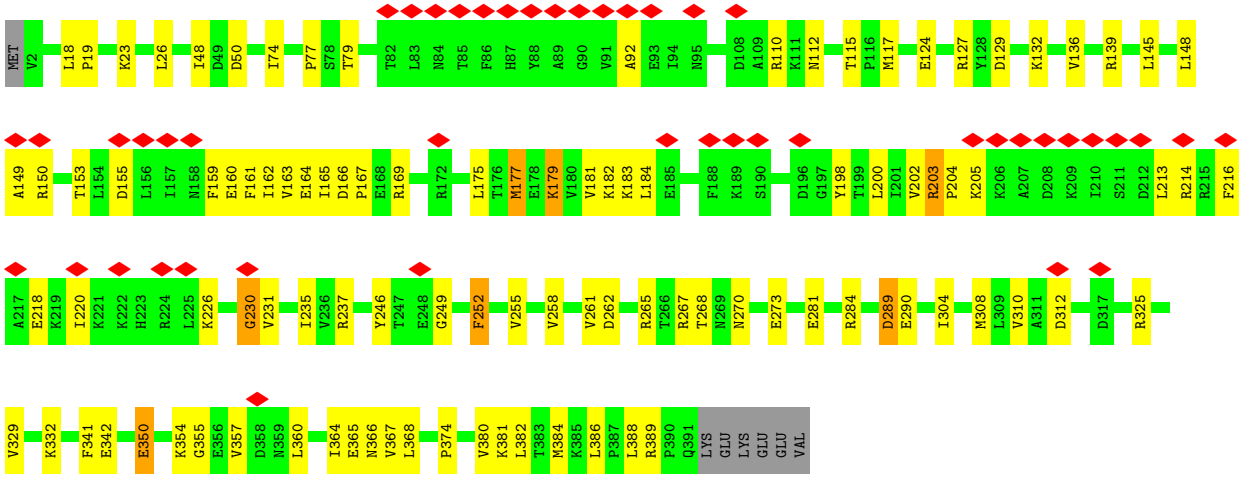
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



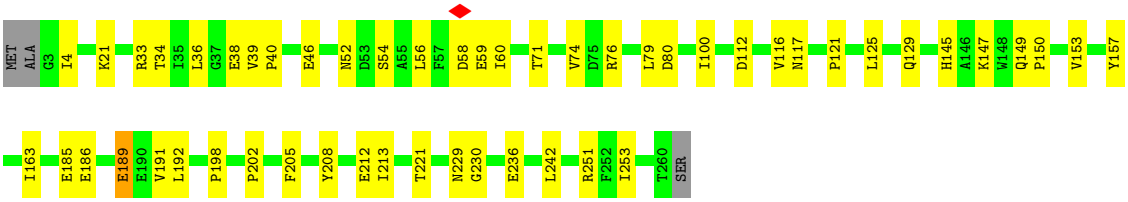
• Molecule 3: DNA-directed RNA polymerase subunit Rpo1C

Chain C:



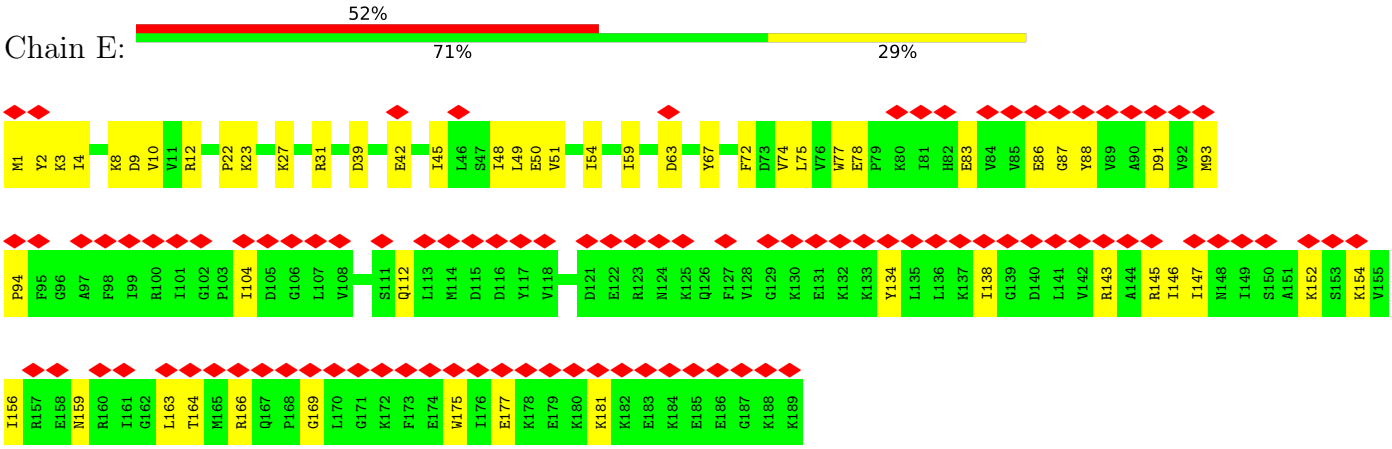
• Molecule 4: DNA-directed RNA polymerase subunit Rpo3

Chain D:



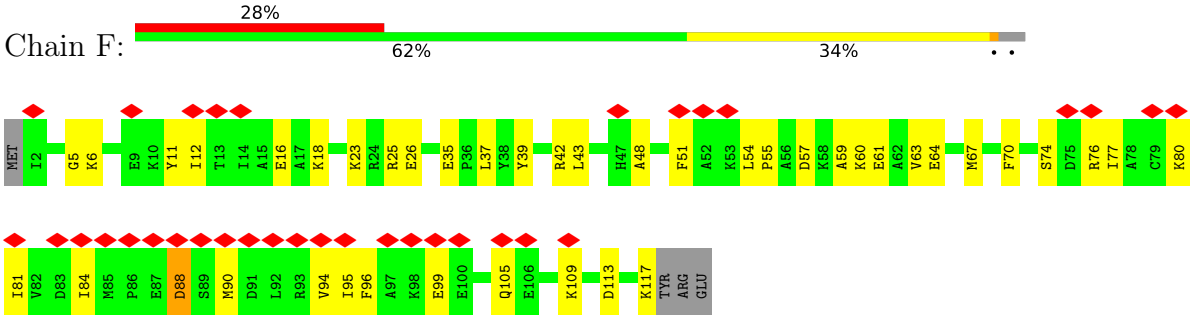
• Molecule 5: DNA-directed RNA polymerase subunit Rpo7

Chain E:



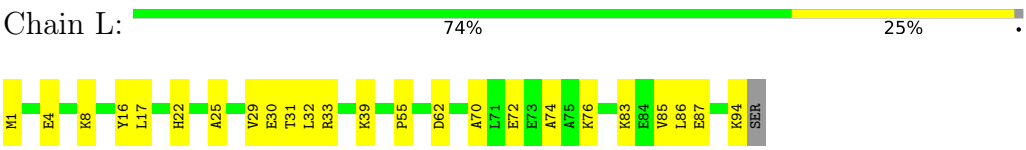
• Molecule 6: DNA-directed RNA polymerase subunit Rpo4

Chain F:



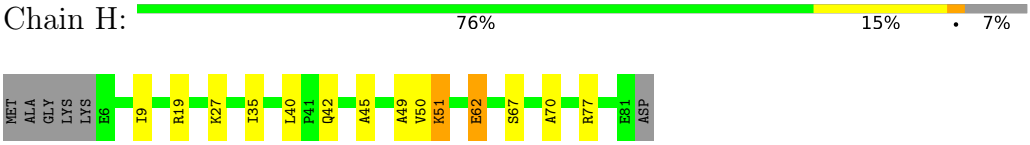
• Molecule 7: DNA-directed RNA polymerase subunit Rpo11

Chain L:



• Molecule 8: DNA-directed RNA polymerase subunit Rpo5

Chain H:

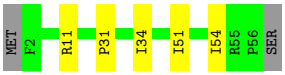


• Molecule 9: DNA-directed RNA polymerase subunit Rpo10

Chain N:

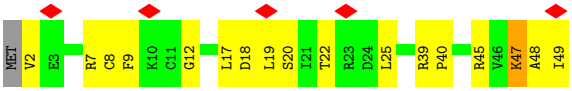
• Molecule 10: DNA-directed RNA polymerase subunit Rpo6

Chain K:



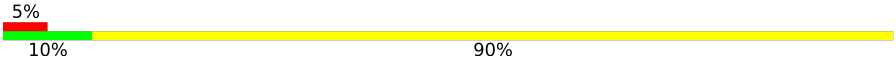
• Molecule 11: DNA-directed RNA polymerase subunit Rpo12

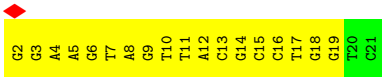
Chain P:



• Molecule 12: DNA Template Strand

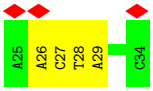
Chain X:





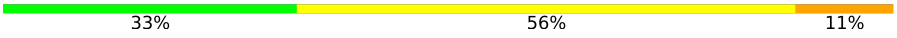
• Molecule 13: DNA Non-Template Strand

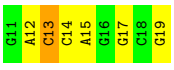
Chain Y:



• Molecule 14: RNA

Chain Z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	333535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	88.73	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	255.24, 255.24, 255.24	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/7330	0.52	0/9897
2	B	0.26	0/8980	0.52	1/12135 (0.0%)
3	C	0.24	0/3098	0.52	1/4180 (0.0%)
4	D	0.26	0/2133	0.45	0/2894
5	E	0.25	0/1556	0.49	0/2091
6	F	0.26	0/959	0.55	0/1284
7	L	0.26	0/792	0.47	0/1067
8	H	0.26	0/622	0.45	0/841
9	N	0.27	0/553	0.50	0/740
10	K	0.26	0/433	0.47	0/588
11	P	0.29	0/400	0.62	0/534
12	X	0.51	0/464	0.90	0/715
13	Y	0.54	0/221	0.96	0/337
14	Z	0.24	0/219	0.83	0/340
All	All	0.27	0/27760	0.53	2/37643 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	230	GLY	O-C-N	-11.75	103.90	122.70
2	B	550	ASP	CB-CG-OD1	5.68	123.41	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	LYS	Peptide
1	A	424	GLN	Peptide
3	C	230	GLY	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7189	0	7251	163	0
2	B	8802	0	8880	179	0
3	C	3057	0	3163	73	0
4	D	2086	0	2109	36	0
5	E	1528	0	1593	36	0
6	F	946	0	961	27	0
7	L	777	0	788	16	0
8	H	609	0	634	9	0
9	N	543	0	541	14	0
10	K	424	0	460	4	0
11	P	393	0	423	13	0
12	X	414	0	226	22	0
13	Y	199	0	114	4	0
14	Z	196	0	99	4	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	N	1	0	0	0	0
15	P	1	0	0	0	0
16	A	1	0	0	0	0
All	All	27169	0	27242	529	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (529) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:CYS:SG	1:A:70:HIS:CE1	2.55	0.92
2:B:1062:CYS:SG	2:B:1080:CYS:HB3	2.21	0.80
3:C:231:VAL:HA	3:C:249:GLY:HA3	1.67	0.76
3:C:268:THR:HG22	3:C:270:ASN:H	1.51	0.75
1:A:483:GLU:OE1	1:A:485:GLN:NE2	2.23	0.72
9:N:36:ASP:OD1	9:N:46:ARG:NH2	2.22	0.71
12:X:5:DA:H2"	12:X:6:DG:H5"	1.70	0.70
12:X:3:DG:H2'	12:X:4:DA:C8	2.27	0.69
11:P:2:VAL:N	11:P:18:ASP:OD2	2.26	0.69
11:P:18:ASP:O	11:P:22:THR:OG1	2.09	0.69
2:B:188:ILE:HD13	2:B:205:GLU:HG3	1.74	0.69
1:A:633:ASP:OD1	1:A:637:ARG:NH1	2.26	0.68
1:A:354:GLU:OE1	1:A:411:ARG:NH1	2.27	0.68
2:B:758:GLU:O	2:B:810:ARG:NH1	2.28	0.67
1:A:832:ARG:NH1	3:C:79:THR:O	2.27	0.67
1:A:345:GLU:OE1	1:A:345:GLU:N	2.26	0.67
1:A:769:GLN:NE2	1:A:770:GLN:O	2.28	0.67
5:E:9:ASP:OD2	5:E:10:VAL:N	2.27	0.67
1:A:670:ASP:OD1	2:B:965:ARG:NH2	2.26	0.67
2:B:580:GLU:OE1	2:B:581:ASN:ND2	2.28	0.67
3:C:202:VAL:HG12	3:C:204:PRO:HD3	1.76	0.67
4:D:208:TYR:HB3	4:D:212:GLU:HB2	1.77	0.66
2:B:27:LEU:HD11	2:B:708:VAL:HG13	1.77	0.66
3:C:267:ARG:NH1	3:C:289:ASP:OD2	2.26	0.66
3:C:175:LEU:HD11	3:C:226:LYS:HG2	1.77	0.66
1:A:492:ARG:HD2	3:C:77:PRO:HG3	1.77	0.66
2:B:899:GLU:HB3	4:D:198:PRO:HG3	1.78	0.65
2:B:566:ASN:ND2	2:B:616:GLU:OE1	2.29	0.65
1:A:335:ILE:O	1:A:448:ASN:ND2	2.30	0.65
1:A:420:LEU:HD11	2:B:1042:LEU:HD21	1.77	0.65
1:A:354:GLU:OE2	1:A:363:ARG:NH2	2.30	0.64
2:B:846:ASP:HB2	2:B:865:ARG:HG2	1.80	0.64
6:F:80:LYS:NZ	6:F:99:GLU:OE2	2.31	0.64
5:E:23:LYS:HD3	5:E:51:VAL:HG23	1.78	0.64
2:B:63:LYS:HB2	2:B:105:ILE:HB	1.78	0.64
7:L:30:GLU:OE1	7:L:33:ARG:NH1	2.31	0.64
1:A:222:ALA:O	1:A:304:ARG:NH2	2.29	0.64
2:B:613:LEU:HD22	2:B:617:GLU:HG2	1.79	0.64
3:C:155:ASP:HB3	3:C:160:GLU:HB2	1.80	0.63
1:A:164:GLU:OE2	1:A:166:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:LYS:HD2	2:B:382:TYR:HE2	1.62	0.63
2:B:179:GLU:HA	2:B:334:GLU:HG2	1.80	0.63
2:B:53:ILE:HG12	2:B:364:VAL:HG13	1.81	0.63
5:E:4:ILE:HG12	6:F:12:ILE:HG21	1.80	0.63
9:N:52:HIS:NE2	9:N:54:GLU:OE1	2.26	0.62
1:A:382:ILE:HB	1:A:408:THR:HB	1.82	0.62
2:B:87:MET:HE1	2:B:684:ARG:HG3	1.81	0.62
2:B:508:GLU:N	2:B:508:GLU:OE2	2.31	0.62
5:E:104:ILE:HD13	5:E:156:ILE:HG22	1.81	0.62
7:L:32:LEU:HD11	7:L:70:ALA:HB1	1.82	0.62
4:D:71:THR:HG23	4:D:116:VAL:HG22	1.81	0.62
2:B:462:ARG:NH2	2:B:618:GLU:OE1	2.31	0.62
1:A:387:ARG:HH21	1:A:389:ARG:HD3	1.63	0.62
4:D:129:GLN:OE1	9:N:63:ARG:NH1	2.33	0.62
2:B:569:ASP:OD1	2:B:570:GLY:N	2.33	0.61
2:B:377:ARG:HH22	2:B:378:LYS:HE3	1.64	0.61
8:H:19:ARG:NH2	8:H:62:GLU:OE2	2.33	0.61
5:E:1:MET:N	5:E:78:GLU:O	2.32	0.61
2:B:440:THR:HG22	2:B:477:VAL:HG22	1.82	0.61
2:B:378:LYS:HD2	2:B:382:TYR:CE2	2.36	0.61
1:A:848:GLN:HG3	3:C:364:ILE:HD11	1.83	0.61
2:B:184:GLN:HB2	2:B:186:LYS:HD2	1.83	0.60
3:C:203:ARG:NH1	3:C:204:PRO:O	2.35	0.60
2:B:122:GLU:N	2:B:122:GLU:OE2	2.35	0.60
7:L:4:GLU:HB2	7:L:16:TYR:HB2	1.84	0.60
2:B:850:ILE:HD12	11:P:19:LEU:HD11	1.83	0.59
6:F:84:ILE:HG21	6:F:95:ILE:HD11	1.83	0.59
6:F:74:SER:H	6:F:77:ILE:HD12	1.66	0.59
5:E:31:ARG:NH1	5:E:48:ILE:O	2.36	0.59
2:B:529:ILE:HD12	2:B:530:GLU:H	1.67	0.59
5:E:169:GLY:HA3	6:F:94:VAL:HG21	1.83	0.59
1:A:875:VAL:HG21	1:A:885:THR:HG23	1.85	0.59
2:B:539:ILE:HG21	2:B:554:VAL:HG21	1.85	0.58
1:A:33:ASP:OD1	1:A:37:TYR:N	2.32	0.58
1:A:343:PRO:HB3	1:A:443:ARG:HA	1.84	0.58
1:A:424:GLN:HE21	12:X:14:DG:H2"	1.68	0.58
1:A:458:ASP:HA	2:B:732:GLU:HG3	1.85	0.58
5:E:22:PRO:HB2	5:E:54:ILE:HD13	1.84	0.58
1:A:545:GLU:OE2	1:A:545:GLU:N	2.36	0.58
2:B:499:LEU:HD11	2:B:565:VAL:HG11	1.85	0.58
3:C:148:LEU:HA	3:C:169:ARG:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ASP:OD2	2:B:417:ARG:NH2	2.36	0.58
5:E:51:VAL:HG12	5:E:72:PHE:HB3	1.87	0.57
12:X:17:DT:H2'	12:X:18:DG:C8	2.39	0.57
1:A:104:LYS:HD2	1:A:151:GLN:HG3	1.87	0.57
1:A:462:ASP:OD1	14:Z:19:G:O2'	2.18	0.57
12:X:10:DT:H2'	12:X:11:DT:C6	2.40	0.57
1:A:97:CYS:O	1:A:186:TRP:NE1	2.37	0.57
2:B:65:GLY:HA3	2:B:103:GLU:HB2	1.86	0.57
3:C:161:PHE:HB3	3:C:202:VAL:HB	1.86	0.57
5:E:83:GLU:H	5:E:146:ILE:HG23	1.69	0.57
2:B:30:GLN:HG2	2:B:31:HIS:N	2.20	0.57
2:B:932:SER:HB2	9:N:43:TYR:HB2	1.86	0.57
1:A:9:GLU:OE2	2:B:1112:ASN:ND2	2.29	0.57
1:A:322:ASN:ND2	2:B:1050:GLU:O	2.38	0.57
4:D:251:ARG:HG3	7:L:1:MET:HG2	1.86	0.57
9:N:57:ASP:HA	9:N:60:MET:HE2	1.86	0.57
2:B:550:ASP:OD1	2:B:573:ARG:NH2	2.32	0.57
2:B:969:TYR:HA	2:B:976:ARG:HA	1.87	0.57
1:A:522:GLU:OE2	1:A:662:LYS:NZ	2.38	0.56
2:B:762:TYR:HE2	2:B:813:PRO:HD2	1.70	0.56
1:A:89:ILE:HD11	1:A:210:MET:HB3	1.88	0.56
1:A:128:ASN:O	1:A:132:LYS:HG3	2.05	0.56
3:C:159:PHE:HA	3:C:213:LEU:HD22	1.87	0.56
12:X:17:DT:H2'	12:X:18:DG:H8	1.70	0.56
1:A:560:LEU:HD21	1:A:654:LEU:HD22	1.86	0.56
2:B:1084:GLU:HG3	2:B:1085:ARG:HG2	1.88	0.56
9:N:1:MET:HA	9:N:55:LEU:HB2	1.87	0.56
3:C:350:GLU:O	3:C:354:LYS:HG3	2.05	0.56
12:X:6:DG:H2'	12:X:7:DT:H71	1.87	0.56
1:A:872:GLU:OE2	3:C:284:ARG:NH2	2.31	0.55
4:D:52:ASN:ND2	4:D:58:ASP:OD1	2.35	0.55
2:B:536:VAL:O	2:B:540:ARG:HG2	2.07	0.55
12:X:15:DC:H2'	12:X:16:DC:H6	1.71	0.55
2:B:695:PRO:HB2	2:B:714:PRO:HG2	1.89	0.55
3:C:115:THR:O	3:C:115:THR:OG1	2.24	0.55
4:D:4:ILE:HG21	7:L:85:VAL:HG22	1.89	0.55
6:F:39:TYR:CZ	6:F:43:LEU:HD11	2.42	0.55
2:B:437:ARG:NH2	2:B:481:ALA:O	2.40	0.55
2:B:939:ASP:OD1	2:B:941:THR:OG1	2.25	0.55
2:B:647:LEU:HB3	2:B:648:PRO:HD3	1.89	0.55
2:B:858:LYS:HE2	11:P:25:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:ARG:NH1	2:B:1021:GLU:O	2.39	0.55
3:C:177:MET:O	3:C:181:VAL:HG23	2.07	0.55
1:A:91:ARG:O	1:A:95:SER:OG	2.21	0.54
4:D:117:ASN:ND2	9:N:16:ASP:OD2	2.39	0.54
5:E:27:LYS:O	5:E:31:ARG:HG2	2.07	0.54
6:F:105:GLN:O	6:F:109:LYS:HG2	2.08	0.54
2:B:336:ASP:O	2:B:342:ASN:ND2	2.39	0.54
5:E:152:LYS:N	5:E:159:ASN:OD1	2.40	0.54
1:A:804:ASN:ND2	1:A:814:GLU:OE1	2.38	0.54
3:C:366:ASN:HD22	3:C:374:PRO:HD3	1.73	0.54
3:C:150:ARG:N	3:C:164:GLU:O	2.40	0.54
4:D:76:ARG:NH1	4:D:112:ASP:OD2	2.41	0.54
6:F:88:ASP:N	6:F:88:ASP:OD1	2.39	0.54
6:F:57:ASP:O	6:F:61:GLU:HG2	2.08	0.53
13:Y:27:DC:H2'	13:Y:28:DT:C6	2.43	0.53
1:A:681:ILE:O	1:A:685:ILE:HD12	2.08	0.53
3:C:386:LEU:HD12	5:E:22:PRO:HB3	1.90	0.53
6:F:16:GLU:OE2	6:F:60:LYS:HE3	2.09	0.53
1:A:717:GLU:O	1:A:721:MET:HG3	2.08	0.53
2:B:496:ARG:NH1	2:B:526:ILE:HG22	2.24	0.53
2:B:1050:GLU:OE1	2:B:1050:GLU:HA	2.08	0.53
4:D:242:LEU:HD13	7:L:86:LEU:HA	1.90	0.53
1:A:320:ARG:NH1	12:X:15:DC:OP1	2.37	0.53
2:B:271:LEU:HD12	2:B:271:LEU:H	1.74	0.53
2:B:554:VAL:HG22	2:B:565:VAL:HG22	1.91	0.53
1:A:654:LEU:O	1:A:658:VAL:HG23	2.08	0.53
2:B:482:LEU:HD13	2:B:704:ILE:HG21	1.91	0.53
2:B:651:LEU:HD23	2:B:670:ALA:HB1	1.91	0.53
2:B:798:GLU:OE1	2:B:865:ARG:NH2	2.41	0.53
2:B:851:THR:OG1	2:B:852:GLU:N	2.41	0.53
1:A:862:GLU:OE2	1:A:862:GLU:N	2.38	0.53
5:E:146:ILE:HA	5:E:163:LEU:HG	1.91	0.53
2:B:298:ASN:N	2:B:298:ASN:HD22	2.06	0.53
2:B:846:ASP:O	11:P:39:ARG:NH2	2.40	0.53
6:F:54:LEU:HD12	6:F:55:PRO:HD2	1.90	0.53
2:B:45:GLU:O	2:B:49:GLU:HG3	2.09	0.52
2:B:510:ARG:NH2	2:B:530:GLU:OE2	2.39	0.52
3:C:150:ARG:HG3	3:C:166:ASP:HB2	1.90	0.52
11:P:8:CYS:SG	11:P:9:PHE:N	2.83	0.52
1:A:673:LEU:O	1:A:678:ARG:NH1	2.43	0.52
4:D:100:ILE:HD11	4:D:121:PRO:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:18:LYS:HG2	6:F:48:ALA:HB1	1.91	0.52
2:B:603:ASP:O	2:B:607:MET:HG3	2.10	0.52
2:B:714:PRO:HG3	9:N:53:VAL:HG21	1.92	0.52
3:C:124:GLU:HA	3:C:127:ARG:HG2	1.92	0.52
3:C:92:ALA:O	3:C:237:ARG:NH2	2.42	0.52
4:D:36:LEU:HD13	4:D:153:VAL:HG12	1.90	0.52
6:F:59:ALA:O	6:F:63:VAL:HG23	2.09	0.52
5:E:177:GLU:O	5:E:181:LYS:HG2	2.10	0.52
2:B:1021:GLU:N	2:B:1021:GLU:OE2	2.43	0.52
3:C:325:ARG:NH1	3:C:342:GLU:OE1	2.32	0.51
1:A:252:LEU:HD13	1:A:268:LEU:HB3	1.92	0.51
1:A:422:ASN:OD1	1:A:424:GLN:HB3	2.11	0.51
1:A:821:GLY:O	1:A:824:GLU:HG3	2.09	0.51
9:N:20:GLU:HG2	9:N:38:LEU:HD21	1.92	0.51
2:B:21:TYR:HB2	2:B:601:TRP:CE3	2.45	0.51
2:B:530:GLU:OE2	2:B:530:GLU:N	2.43	0.51
3:C:149:ALA:O	3:C:169:ARG:NH1	2.43	0.51
2:B:577:ILE:HD11	2:B:639:LEU:HD13	1.93	0.51
3:C:289:ASP:OD1	3:C:290:GLU:N	2.44	0.51
3:C:360:LEU:HA	3:C:365:GLU:HG3	1.92	0.51
12:X:12:DA:H2'	12:X:13:DC:H6	1.76	0.51
1:A:570:ARG:NH2	1:A:581:GLU:OE2	2.43	0.51
2:B:265:THR:HG23	2:B:269:GLU:HG2	1.91	0.51
2:B:441:SER:O	2:B:445:ARG:NH2	2.44	0.51
1:A:853:GLU:HG3	1:A:859:ARG:HD2	1.92	0.51
6:F:96:PHE:HA	6:F:99:GLU:HG3	1.91	0.51
2:B:655:PRO:HD2	2:B:942:ALA:HA	1.93	0.51
5:E:49:LEU:HD21	5:E:75:LEU:HB2	1.93	0.51
1:A:523:VAL:O	1:A:526:MET:HG2	2.11	0.50
1:A:865:ILE:HD11	8:H:35:ILE:HG21	1.94	0.50
2:B:310:ARG:HA	2:B:313:LYS:HD2	1.94	0.50
12:X:12:DA:H2'	12:X:13:DC:C6	2.46	0.50
1:A:253:LYS:O	1:A:257:GLU:HG3	2.10	0.50
2:B:880:HIS:NE2	2:B:924:GLU:OE1	2.41	0.50
12:X:13:DC:H2'	12:X:14:DG:C8	2.47	0.50
3:C:153:THR:HB	3:C:162:ILE:HB	1.94	0.50
13:Y:26:DA:H2"	13:Y:27:DC:O5'	2.12	0.50
1:A:212:LEU:HD23	1:A:212:LEU:H	1.77	0.50
1:A:168:ASP:HB3	1:A:174:TYR:CD1	2.47	0.49
1:A:802:VAL:HA	1:A:814:GLU:HG2	1.93	0.49
1:A:806:TYR:OH	1:A:818:HIS:NE2	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:21:LYS:NZ	4:D:221:THR:OG1	2.45	0.49
4:D:46:GLU:HG2	11:P:45:ARG:HD2	1.93	0.49
1:A:393:ASP:O	1:A:394:SER:OG	2.26	0.49
2:B:230:ARG:NH1	2:B:237:ASP:OD2	2.40	0.49
4:D:74:VAL:HG11	4:D:236:GLU:HG2	1.94	0.49
1:A:672:ASP:OD2	1:A:807:LYS:NZ	2.31	0.49
2:B:169:GLU:OE2	2:B:340:TYR:OH	2.30	0.49
2:B:377:ARG:HH11	2:B:377:ARG:HG2	1.76	0.49
2:B:553:ASN:HB2	2:B:571:ARG:HH12	1.77	0.49
5:E:87:GLY:HA2	6:F:51:PHE:CZ	2.48	0.49
2:B:515:THR:HG23	2:B:516:LEU:HD12	1.94	0.49
2:B:81:ARG:HH21	2:B:119:ARG:CZ	2.26	0.49
5:E:39:ASP:OD2	5:E:42:GLU:N	2.43	0.49
2:B:68:ARG:NH2	2:B:117:GLU:OE2	2.35	0.49
2:B:1097:LEU:O	2:B:1101:GLU:HG3	2.13	0.49
1:A:185:ASP:HA	1:A:188:GLU:HG3	1.94	0.49
1:A:748:MET:SD	2:B:914:PRO:HG3	2.53	0.49
2:B:868:ARG:NH1	2:B:994:MET:SD	2.86	0.49
3:C:284:ARG:NE	3:C:312:ASP:OD1	2.44	0.49
4:D:163:ILE:HA	4:D:213:ILE:HG22	1.94	0.49
1:A:728:ARG:HD3	1:A:768:GLY:HA3	1.95	0.49
4:D:229:ASN:HD22	9:N:6:ARG:HH21	1.61	0.49
1:A:341:GLY:HA3	1:A:446:ARG:HB2	1.95	0.48
2:B:875:LYS:HD3	2:B:991:LEU:HD12	1.95	0.48
1:A:82:HIS:CE1	1:A:280:ILE:HD13	2.48	0.48
2:B:13:ASP:HB3	2:B:591:VAL:HG11	1.95	0.48
2:B:543:ARG:NH2	2:B:611:GLU:OE2	2.43	0.48
1:A:501:ILE:HG13	1:A:502:GLN:H	1.76	0.48
3:C:380:VAL:HB	10:K:11:ARG:HG3	1.94	0.48
4:D:116:VAL:HG11	4:D:230:GLY:HA3	1.95	0.48
1:A:9:GLU:HG2	3:C:357:VAL:HG12	1.95	0.48
2:B:325:ILE:O	2:B:329:LEU:HG	2.14	0.48
1:A:43:VAL:HG21	1:A:239:THR:HG23	1.95	0.48
1:A:773:ARG:HG3	1:A:773:ARG:HH11	1.79	0.48
2:B:237:ASP:O	2:B:241:VAL:HG23	2.13	0.48
1:A:370:ASN:HD22	1:A:376:PRO:HG2	1.78	0.48
1:A:873:ASP:HB3	8:H:70:ALA:HB2	1.95	0.48
5:E:86:GLU:OE2	5:E:143:ARG:NE	2.43	0.48
3:C:18:LEU:O	3:C:23:LYS:NZ	2.42	0.48
3:C:150:ARG:H	3:C:165:ILE:HA	1.78	0.48
1:A:815:TYR:HE2	2:B:645:LEU:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:39:TYR:O	6:F:43:LEU:HG	2.14	0.48
2:B:80:GLN:OE1	2:B:80:GLN:N	2.47	0.47
7:L:31:THR:HG23	7:L:74:ALA:HB1	1.96	0.47
12:X:15:DC:H2'	12:X:16:DC:C6	2.49	0.47
2:B:178:VAL:HB	2:B:327:LEU:HD22	1.96	0.47
2:B:300:LEU:HB2	2:B:313:LYS:HG2	1.95	0.47
1:A:889:ASP:OD1	1:A:889:ASP:N	2.44	0.47
9:N:16:ASP:N	9:N:16:ASP:OD1	2.45	0.47
1:A:423:ARG:HB2	1:A:464:MET:HE3	1.96	0.47
2:B:753:ARG:NH1	12:X:18:DG:OP1	2.34	0.47
1:A:97:CYS:HA	1:A:151:GLN:OE1	2.14	0.47
2:B:187:TYR:CZ	2:B:328:SER:HA	2.50	0.47
3:C:255:VAL:O	3:C:261:VAL:HG21	2.15	0.47
3:C:329:VAL:HG11	3:C:341:PHE:CD2	2.50	0.47
1:A:429:ARG:HA	2:B:1033:VAL:HG13	1.97	0.47
5:E:112:GLN:O	5:E:166:ARG:HG3	2.14	0.47
11:P:7:ARG:NH1	11:P:12:GLY:O	2.41	0.47
1:A:166:ARG:NH2	1:A:174:TYR:OH	2.40	0.47
1:A:523:VAL:HA	1:A:526:MET:SD	2.55	0.47
1:A:685:ILE:O	1:A:689:GLU:HG3	2.15	0.47
1:A:707:LEU:HG	1:A:715:THR:HG23	1.97	0.47
3:C:252:PHE:N	3:C:273:GLU:OE2	2.42	0.47
3:C:304:ILE:O	3:C:308:MET:HG3	2.15	0.47
5:E:4:ILE:HD12	5:E:49:LEU:HD11	1.96	0.47
6:F:25:ARG:HG2	6:F:25:ARG:HH11	1.80	0.47
6:F:76:ARG:O	6:F:80:LYS:HG2	2.14	0.47
1:A:642:GLU:OE1	1:A:645:ARG:NH1	2.47	0.47
1:A:772:ILE:O	1:A:772:ILE:HG13	2.15	0.47
4:D:147:LYS:NZ	11:P:48:ALA:O	2.30	0.47
5:E:63:ASP:OD1	5:E:63:ASP:N	2.46	0.47
7:L:32:LEU:HD13	7:L:74:ALA:HB2	1.97	0.47
1:A:510:LEU:HD11	1:A:664:PHE:CD1	2.49	0.46
2:B:321:ALA:O	2:B:325:ILE:HG13	2.14	0.46
2:B:853:THR:HG23	2:B:859:LEU:HB2	1.97	0.46
1:A:489:ILE:HD11	1:A:636:VAL:HG11	1.97	0.46
2:B:743:GLU:HB3	4:D:145:HIS:CE1	2.50	0.46
5:E:134:TYR:HB3	5:E:175:TRP:CZ2	2.50	0.46
1:A:206:ARG:HB2	1:A:209:TRP:CD2	2.50	0.46
1:A:895:THR:O	1:A:899:MET:HG3	2.15	0.46
2:B:447:GLN:OE1	2:B:447:GLN:N	2.49	0.46
2:B:99:PRO:HB3	2:B:119:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:ILE:HD11	2:B:203:ALA:HB1	1.97	0.46
2:B:139:ASP:N	2:B:139:ASP:OD1	2.48	0.46
1:A:872:GLU:OE1	8:H:67:SER:OG	2.22	0.46
2:B:536:VAL:HG21	2:B:556:TYR:HB3	1.98	0.46
2:B:539:ILE:HG21	2:B:554:VAL:CG2	2.45	0.46
1:A:820:MET:HG2	2:B:455:LEU:HB3	1.98	0.46
4:D:40:PRO:HG2	4:D:79:LEU:HD22	1.98	0.46
9:N:33:LYS:HB2	9:N:33:LYS:HE2	1.70	0.46
2:B:205:GLU:N	2:B:213:TYR:O	2.48	0.46
2:B:647:LEU:HD11	2:B:708:VAL:HG11	1.98	0.46
3:C:181:VAL:HG22	3:C:200:LEU:HD12	1.98	0.46
2:B:54:LYS:O	2:B:54:LYS:HG3	2.16	0.46
2:B:225:PHE:CE1	2:B:321:ALA:HB2	2.51	0.46
4:D:186:GLU:HA	4:D:191:VAL:HA	1.98	0.46
6:F:35:GLU:OE2	6:F:42:ARG:NE	2.41	0.46
8:H:51:LYS:HE3	8:H:51:LYS:HA	1.96	0.46
14:Z:12:A:HO2'	14:Z:13:C:H6	1.59	0.46
1:A:56:ARG:HA	1:A:56:ARG:HD3	1.62	0.46
1:A:575:ASP:OD2	1:A:750:LYS:NZ	2.49	0.46
2:B:18:MET:HG2	2:B:639:LEU:HG	1.98	0.46
3:C:382:LEU:HB2	5:E:59:ILE:HB	1.98	0.46
1:A:518:PHE:HE1	1:A:662:LYS:HE3	1.81	0.45
2:B:241:VAL:HG12	2:B:251:GLN:OE1	2.16	0.45
2:B:724:LEU:HD23	2:B:981:ILE:HG21	1.98	0.45
4:D:185:GLU:O	4:D:192:LEU:N	2.39	0.45
11:P:18:ASP:OD1	11:P:20:SER:N	2.49	0.45
2:B:542:ASP:OD1	2:B:547:LYS:HB2	2.17	0.45
2:B:1104:ALA:O	2:B:1105:MET:HG2	2.16	0.45
2:B:72:PRO:HG3	2:B:125:ILE:HD12	1.98	0.45
1:A:158:LYS:HB3	1:A:159:PRO:HD3	1.98	0.45
2:B:227:TYR:CE1	2:B:265:THR:HB	2.52	0.45
2:B:687:THR:OG1	12:X:19:DG:OP1	2.34	0.45
3:C:384:MET:HE2	3:C:388:LEU:HD21	1.99	0.45
12:X:18:DG:H2"	12:X:19:DG:H8	1.80	0.45
1:A:97:CYS:HB3	1:A:101:GLY:H	1.80	0.45
1:A:898:LYS:HE3	1:A:898:LYS:HB3	1.75	0.45
2:B:806:VAL:HA	2:B:836:ALA:HA	1.97	0.45
3:C:136:VAL:HG12	3:C:139:ARG:NH2	2.32	0.45
1:A:423:ARG:NH1	14:Z:19:G:O2'	2.49	0.45
2:B:66:LYS:HE3	2:B:66:LYS:HB2	1.69	0.45
2:B:229:MET:HG2	2:B:240:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLN:HG2	1:A:17:GLU:N	2.32	0.45
1:A:72:GLY:O	1:A:217:VAL:N	2.35	0.45
1:A:167:LYS:HA	1:A:173:GLU:HA	1.99	0.45
1:A:830:ALA:O	1:A:833:THR:HG22	2.17	0.45
2:B:15:TRP:HZ3	2:B:22:TRP:HZ3	1.64	0.45
1:A:711:SER:OG	1:A:712:LEU:N	2.49	0.45
2:B:1059:CYS:HB2	2:B:1077:CYS:HB2	1.99	0.45
1:A:152:TYR:HB3	1:A:165:ILE:O	2.16	0.45
2:B:489:ALA:HB2	2:B:569:ASP:HB2	1.99	0.45
2:B:801:VAL:HG23	2:B:805:ASP:HB2	1.99	0.45
2:B:626:TRP:HB2	2:B:629:GLU:HG3	1.98	0.44
2:B:848:VAL:HG13	2:B:862:VAL:HG22	1.99	0.44
5:E:3:LYS:HE2	6:F:11:TYR:CE1	2.53	0.44
1:A:108:GLU:O	1:A:111:GLU:HG2	2.17	0.44
2:B:536:VAL:HG13	2:B:554:VAL:HG12	1.99	0.44
7:L:25:ALA:O	7:L:29:VAL:HG22	2.17	0.44
2:B:28:VAL:HG11	2:B:436:LEU:HD13	1.99	0.44
2:B:237:ASP:HB3	2:B:258:LEU:HD11	1.99	0.44
2:B:954:GLU:O	2:B:957:GLU:HG2	2.17	0.44
5:E:147:ILE:HD13	5:E:164:THR:HB	1.99	0.44
1:A:10:PHE:O	3:C:355:GLY:HA2	2.17	0.44
2:B:814:PRO:HB3	2:B:829:GLU:O	2.17	0.44
4:D:125:LEU:HD22	4:D:129:GLN:HB3	1.98	0.44
1:A:159:PRO:HD3	1:A:285:PRO:O	2.17	0.44
1:A:375:TYR:O	1:A:412:HIS:ND1	2.35	0.44
1:A:411:ARG:HH21	1:A:414:MET:HG2	1.81	0.44
1:A:511:LEU:HD12	1:A:518:PHE:CE2	2.53	0.44
1:A:511:LEU:O	1:A:553:GLY:HA3	2.18	0.44
1:A:512:THR:HG21	1:A:619:ILE:HG12	2.00	0.44
2:B:899:GLU:HG3	2:B:969:TYR:HE1	1.81	0.44
5:E:93:MET:HG3	5:E:94:PRO:HD2	1.99	0.44
2:B:976:ARG:HH21	4:D:157:TYR:HB2	1.82	0.44
3:C:145:LEU:HD21	3:C:163:VAL:HG21	2.00	0.44
4:D:202:PRO:HG2	4:D:205:PHE:HD2	1.82	0.44
5:E:91:ASP:HA	5:E:138:ILE:HG12	2.00	0.44
6:F:6:LYS:HE3	6:F:6:LYS:HB2	1.82	0.44
1:A:136:LYS:HB3	1:A:136:LYS:HE2	1.76	0.44
1:A:370:ASN:ND2	1:A:376:PRO:HG2	2.32	0.44
1:A:453:PRO:HB3	1:A:626:ARG:HH11	1.83	0.44
1:A:477:GLU:OE1	2:B:1041:MET:N	2.51	0.44
2:B:14:LEU:HB3	2:B:639:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:ALA:O	2:B:324:VAL:HG12	2.18	0.44
4:D:34:THR:O	4:D:38:GLU:HB2	2.18	0.44
1:A:93:LEU:HD11	1:A:183:VAL:HG22	1.98	0.44
1:A:261:PRO:HG2	1:A:264:ILE:HD12	2.00	0.44
2:B:377:ARG:HG2	2:B:377:ARG:NH1	2.32	0.44
4:D:59:GLU:H	4:D:59:GLU:HG2	1.66	0.44
7:L:76:LYS:HD2	7:L:76:LYS:HA	1.75	0.44
8:H:9:ILE:HD11	8:H:49:ALA:HA	1.99	0.44
1:A:485:GLN:H	1:A:485:GLN:HG3	1.61	0.43
5:E:8:LYS:HE2	6:F:5:GLY:HA3	1.99	0.43
1:A:158:LYS:HB3	1:A:159:PRO:CD	2.48	0.43
1:A:427:LEU:O	1:A:840:GLN:NE2	2.50	0.43
2:B:744:ARG:NH2	4:D:149:GLN:OE1	2.51	0.43
6:F:77:ILE:HA	6:F:80:LYS:HE3	2.01	0.43
1:A:104:LYS:HA	1:A:145:PRO:HD2	1.99	0.43
1:A:316:LEU:O	1:A:319:LYS:NZ	2.51	0.43
1:A:784:ARG:NH2	2:B:619:GLU:O	2.51	0.43
2:B:762:TYR:CE2	2:B:813:PRO:HD2	2.52	0.43
3:C:74:ILE:HD12	3:C:310:VAL:HG21	2.01	0.43
3:C:129:ASP:HB3	3:C:132:LYS:HG3	2.00	0.43
3:C:262:ASP:OD2	3:C:265:ARG:NH1	2.42	0.43
3:C:381:LYS:HB2	10:K:54:ILE:HG12	2.00	0.43
2:B:396:ARG:CZ	2:B:396:ARG:HB2	2.48	0.43
12:X:2:DG:H3'	12:X:3:DG:H8	1.83	0.43
1:A:424:GLN:HE21	12:X:14:DG:C2'	2.31	0.43
2:B:671:LYS:HB2	2:B:671:LYS:HE2	1.82	0.43
2:B:1052:ASP:OD1	2:B:1052:ASP:N	2.50	0.43
4:D:56:LEU:HD22	4:D:60:ILE:HG21	2.00	0.43
1:A:773:ARG:HG3	1:A:773:ARG:NH1	2.33	0.43
3:C:364:ILE:O	3:C:368:LEU:HG	2.17	0.43
1:A:418:ILE:HD11	1:A:434:ALA:HB1	2.00	0.43
4:D:33:ARG:NH2	7:L:22:HIS:HB2	2.34	0.43
5:E:175:TRP:CD1	5:E:175:TRP:N	2.86	0.43
12:X:16:DC:H2'	12:X:17:DT:C6	2.54	0.43
1:A:291:LYS:HA	1:A:297:PRO:HA	2.01	0.43
1:A:432:ILE:HG13	2:B:1033:VAL:HG11	2.01	0.43
2:B:487:THR:HB	2:B:551:VAL:HG13	2.00	0.43
3:C:214:ARG:O	3:C:218:GLU:HG2	2.19	0.43
3:C:235:ILE:HG12	3:C:246:TYR:HB2	2.00	0.43
4:D:80:ASP:OD1	4:D:80:ASP:N	2.47	0.43
12:X:16:DC:H2'	12:X:17:DT:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HD23	1:A:120:ALA:HB2	2.01	0.43
1:A:387:ARG:HE	1:A:389:ARG:HD3	1.84	0.43
1:A:637:ARG:NH2	1:A:880:SER:O	2.51	0.43
3:C:255:VAL:O	3:C:258:VAL:HG22	2.19	0.43
12:X:8:DA:H2"	12:X:9:DG:H8	1.84	0.43
2:B:370:GLN:CD	2:B:396:ARG:HH21	2.22	0.43
2:B:428:ASN:ND2	2:B:673:SER:O	2.49	0.43
2:B:548:ILE:HD13	2:B:548:ILE:HA	1.81	0.43
2:B:555:ALA:HB2	2:B:617:GLU:HA	2.01	0.43
7:L:17:LEU:O	7:L:55:PRO:HD2	2.18	0.43
11:P:47:LYS:HG2	11:P:49:ILE:HG22	2.01	0.43
1:A:117:ILE:HD13	1:A:117:ILE:HA	1.79	0.42
5:E:2:TYR:CD1	5:E:77:TRP:HD1	2.37	0.42
3:C:145:LEU:HD22	3:C:220:ILE:HG22	2.01	0.42
2:B:47:VAL:HG21	2:B:67:ILE:HG13	2.02	0.42
2:B:50:PHE:CZ	2:B:361:SER:HB2	2.55	0.42
2:B:211:ILE:HD12	2:B:211:ILE:HA	1.85	0.42
2:B:701:ASN:ND2	2:B:711:GLU:OE1	2.53	0.42
4:D:189:GLU:OE1	4:D:189:GLU:N	2.51	0.42
5:E:12:ARG:HG3	5:E:67:TYR:CZ	2.54	0.42
1:A:518:PHE:CE1	1:A:662:LYS:HE3	2.55	0.42
1:A:527:LEU:HD13	1:A:534:ILE:HD13	2.01	0.42
1:A:570:ARG:NH2	1:A:584:GLU:OE2	2.53	0.42
3:C:26:LEU:HD21	3:C:48:ILE:HD13	2.01	0.42
1:A:195:LEU:HD12	1:A:202:PRO:HA	2.01	0.42
1:A:315:ASN:O	1:A:319:LYS:HE3	2.20	0.42
1:A:429:ARG:O	2:B:1037:HIS:NE2	2.52	0.42
2:B:226:VAL:O	2:B:230:ARG:HG3	2.20	0.42
7:L:83:LYS:O	7:L:87:GLU:HG2	2.18	0.42
2:B:311:ILE:HG12	2:B:315:TYR:CE1	2.55	0.42
2:B:879:ARG:NH2	2:B:924:GLU:OE2	2.52	0.42
3:C:268:THR:HG22	3:C:270:ASN:N	2.28	0.42
3:C:386:LEU:HD23	3:C:386:LEU:HA	1.77	0.42
8:H:40:LEU:HD23	8:H:40:LEU:HA	1.93	0.42
1:A:312:PHE:HA	1:A:316:LEU:HD12	2.02	0.42
1:A:453:PRO:HB3	1:A:626:ARG:HD2	2.02	0.42
1:A:772:ILE:HD12	1:A:773:ARG:NH2	2.35	0.42
2:B:804:LYS:HB2	2:B:804:LYS:HE3	1.83	0.42
3:C:19:PRO:O	3:C:23:LYS:HG3	2.19	0.42
3:C:389:ARG:HD3	3:C:389:ARG:HA	1.78	0.42
4:D:52:ASN:OD1	4:D:54:SER:OG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:23:LYS:O	6:F:26:GLU:HG3	2.19	0.42
6:F:81:ILE:HD11	6:F:96:PHE:HZ	1.85	0.42
1:A:26:VAL:HG21	1:A:48:MET:HE1	2.02	0.41
1:A:470:GLN:HG3	2:B:1050:GLU:OE2	2.19	0.41
2:B:57:ILE:HG13	2:B:60:PHE:HD2	1.83	0.41
11:P:19:LEU:HG	11:P:25:LEU:HD21	2.01	0.41
1:A:363:ARG:O	1:A:367:MET:HG3	2.20	0.41
1:A:845:ASN:O	3:C:332:LYS:NZ	2.43	0.41
2:B:336:ASP:HB3	2:B:339:HIS:HB2	2.01	0.41
2:B:697:ILE:HG12	9:N:53:VAL:HG22	2.01	0.41
2:B:850:ILE:HG22	2:B:860:VAL:HG12	2.02	0.41
3:C:177:MET:SD	3:C:177:MET:N	2.85	0.41
14:Z:14:C:H2'	14:Z:15:A:C8	2.56	0.41
1:A:150:PRO:O	1:A:151:GLN:NE2	2.53	0.41
1:A:328:VAL:O	1:A:444:THR:OG1	2.30	0.41
2:B:29:ARG:O	2:B:33:ASP:HB2	2.20	0.41
4:D:39:VAL:HB	4:D:150:PRO:HG3	2.01	0.41
1:A:283:GLU:OE1	1:A:303:GLN:NE2	2.54	0.41
1:A:284:ALA:O	1:A:287:VAL:HG12	2.20	0.41
2:B:129:SER:O	2:B:135:TYR:HB2	2.19	0.41
3:C:182:LYS:HG3	3:C:183:LYS:N	2.35	0.41
3:C:184:LEU:HD21	3:C:220:ILE:HG23	2.01	0.41
1:A:573:LEU:HD21	1:A:751:THR:HG22	2.02	0.41
1:A:607:VAL:HA	1:A:617:GLY:HA3	2.02	0.41
1:A:763:MET:HG3	2:B:917:MET:HG2	2.03	0.41
4:D:253:ILE:HG12	7:L:72:GLU:OE1	2.21	0.41
1:A:649:ASP:OD1	1:A:653:LYS:NZ	2.39	0.41
2:B:961:LYS:HA	2:B:961:LYS:HD3	1.77	0.41
3:C:167:PRO:HB3	3:C:198:TYR:CZ	2.56	0.41
5:E:83:GLU:O	5:E:145:ARG:HG3	2.20	0.41
5:E:154:LYS:HB3	5:E:154:LYS:HE3	1.85	0.41
1:A:94:GLU:OE1	1:A:135:HIS:NE2	2.45	0.41
1:A:158:LYS:HA	1:A:158:LYS:HD2	1.71	0.41
1:A:339:GLU:HG2	1:A:436:ARG:HB2	2.02	0.41
2:B:562:GLU:OE1	2:B:564:TYR:OH	2.22	0.41
2:B:931:ALA:HB2	2:B:938:VAL:HG23	2.03	0.41
2:B:633:GLU:OE1	2:B:633:GLU:N	2.54	0.41
2:B:868:ARG:NH2	2:B:997:ASP:OD1	2.54	0.41
1:A:338:ASN:HA	1:A:484:VAL:HB	2.01	0.41
2:B:127:LEU:HD11	2:B:157:ILE:HD12	2.03	0.41
3:C:258:VAL:O	3:C:261:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:281:GLU:OE2	8:H:77:ARG:NE	2.50	0.41
3:C:341:PHE:CD2	3:C:342:GLU:HG3	2.56	0.41
5:E:104:ILE:HD12	5:E:104:ILE:HA	1.94	0.41
12:X:4:DA:H2"	12:X:5:DA:H5"	2.03	0.41
2:B:676:LEU:HD22	9:N:55:LEU:HD22	2.03	0.41
2:B:796:PHE:HB3	11:P:40:PRO:HG3	2.02	0.41
3:C:110:ARG:NH1	13:Y:28:DT:O5'	2.53	0.41
3:C:184:LEU:HD11	3:C:220:ILE:HG23	2.02	0.41
1:A:418:ILE:HD13	1:A:479:ARG:HG3	2.03	0.40
1:A:449:LEU:HG	2:B:731:MET:SD	2.60	0.40
1:A:556:ILE:N	1:A:556:ILE:HD13	2.37	0.40
1:A:831:VAL:HG11	2:B:450:PHE:HZ	1.86	0.40
3:C:179:LYS:HA	3:C:182:LYS:HG2	2.03	0.40
5:E:45:ILE:HG23	5:E:74:VAL:HG21	2.02	0.40
13:Y:28:DT:H2'	13:Y:29:DA:C8	2.56	0.40
1:A:204:LYS:HE3	1:A:204:LYS:HB2	1.93	0.40
1:A:435:HIS:CE1	1:A:484:VAL:HG21	2.56	0.40
1:A:690:GLU:HG2	1:A:694:LYS:HE3	2.03	0.40
1:A:754:ARG:HG2	2:B:911:HIS:O	2.20	0.40
2:B:999:ILE:O	2:B:1018:ARG:NH1	2.54	0.40
3:C:182:LYS:HG3	3:C:183:LYS:H	1.84	0.40
7:L:39:LYS:HD3	7:L:62:ASP:HA	2.02	0.40
10:K:31:PRO:HD2	10:K:34:ILE:HG13	2.03	0.40
1:A:323:PHE:HA	1:A:350:LEU:HD22	2.04	0.40
1:A:825:GLY:O	1:A:829:THR:HG23	2.20	0.40
1:A:847:LEU:HD11	3:C:310:VAL:HG22	2.02	0.40
3:C:166:ASP:HB3	3:C:169:ARG:HE	1.86	0.40
1:A:443:ARG:H	1:A:443:ARG:HG2	1.72	0.40
2:B:224:LYS:HE2	2:B:224:LYS:HB2	1.92	0.40
2:B:1031:ARG:HD3	3:C:367:VAL:HG11	2.04	0.40
3:C:382:LEU:HD13	10:K:51:ILE:HG21	2.04	0.40
6:F:90:MET:O	6:F:94:VAL:HG23	2.22	0.40
6:F:113:ASP:O	6:F:117:LYS:HE3	2.21	0.40
7:L:8:LYS:HD2	7:L:8:LYS:HA	1.96	0.40
8:H:45:ALA:HA	8:H:50:VAL:HG11	2.02	0.40
1:A:381:VAL:HG23	1:A:391:ILE:HD11	2.04	0.40
2:B:717:GLN:HB2	2:B:719:PHE:HE1	1.86	0.40
2:B:1056:VAL:HG11	2:B:1065:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	898/910 (99%)	882 (98%)	16 (2%)	0	100	100
2	B	1094/1117 (98%)	1077 (98%)	17 (2%)	0	100	100
3	C	388/397 (98%)	382 (98%)	6 (2%)	0	100	100
4	D	256/261 (98%)	254 (99%)	2 (1%)	0	100	100
5	E	187/189 (99%)	182 (97%)	5 (3%)	0	100	100
6	F	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
7	L	92/95 (97%)	89 (97%)	3 (3%)	0	100	100
8	H	74/82 (90%)	73 (99%)	1 (1%)	0	100	100
9	N	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
10	K	53/57 (93%)	52 (98%)	1 (2%)	0	100	100
11	P	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
All	All	3265/3342 (98%)	3209 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	776/785 (99%)	764 (98%)	12 (2%)	65	85
2	B	946/962 (98%)	926 (98%)	20 (2%)	53	79
3	C	338/345 (98%)	327 (97%)	11 (3%)	38	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	230/232 (99%)	229 (100%)	1 (0%)	91 96
5	E	167/167 (100%)	165 (99%)	2 (1%)	71 88
6	F	99/103 (96%)	94 (95%)	5 (5%)	24 56
7	L	83/84 (99%)	82 (99%)	1 (1%)	71 88
8	H	66/70 (94%)	62 (94%)	4 (6%)	18 49
9	N	60/60 (100%)	58 (97%)	2 (3%)	38 69
10	K	45/47 (96%)	45 (100%)	0	100 100
11	P	44/45 (98%)	42 (96%)	2 (4%)	27 60
All	All	2854/2900 (98%)	2794 (98%)	60 (2%)	56 79

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	CYS
1	A	125	SER
1	A	163	TRP
1	A	185	ASP
1	A	236	ASP
1	A	237	ASP
1	A	306	LYS
1	A	375	TYR
1	A	411	ARG
1	A	415	ASP
1	A	503	ASP
1	A	544	ASP
2	B	18	MET
2	B	139	ASP
2	B	271	LEU
2	B	297	ASN
2	B	298	ASN
2	B	377	ARG
2	B	400	LEU
2	B	413	TRP
2	B	494	GLU
2	B	568	ASP
2	B	756	GLU
2	B	810	ARG
2	B	831	ARG
2	B	851	THR

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Mol	Chain	Res	Type
2	B	975	LYS
2	B	992	HIS
2	B	1067	LEU
2	B	1073	ARG
2	B	1080	CYS
2	B	1116	ARG
3	C	50	ASP
3	C	112	ASN
3	C	117	MET
3	C	177	MET
3	C	179	LYS
3	C	203	ARG
3	C	205	LYS
3	C	216	PHE
3	C	252	PHE
3	C	289	ASP
3	C	350	GLU
4	D	189	GLU
5	E	50	GLU
5	E	88	TYR
6	F	37	LEU
6	F	64	GLU
6	F	67	MET
6	F	70	PHE
6	F	88	ASP
7	L	94	LYS
8	H	27	LYS
8	H	42	GLN
8	H	51	LYS
8	H	62	GLU
9	N	23	ARG
9	N	37	ASP
11	P	17	LEU
11	P	47	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	GLN
1	A	465	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	Z	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	Z	13	C
14	Z	17	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

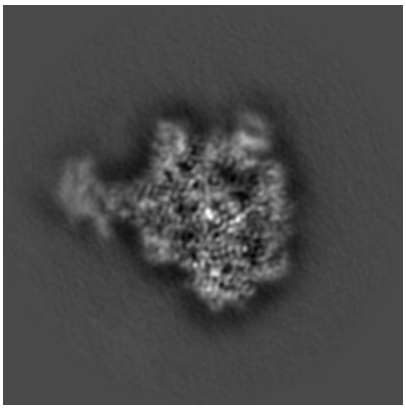
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16809. These allow visual inspection of the internal detail of the map and identification of artifacts.

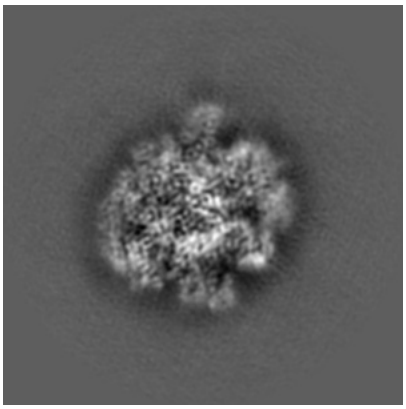
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

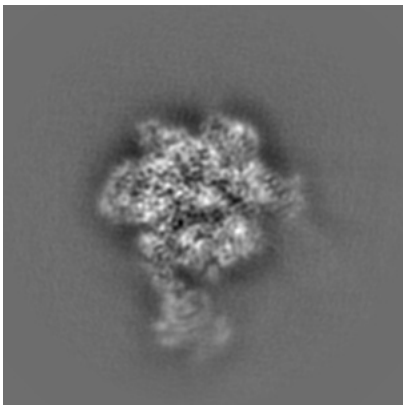
6.1.1 Primary map



X

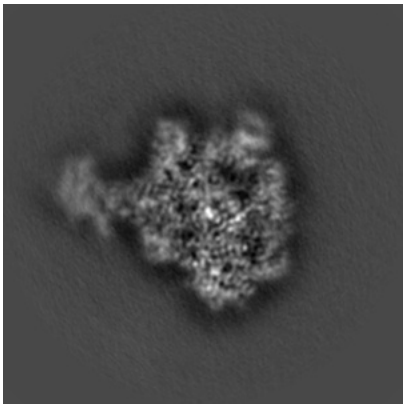


Y

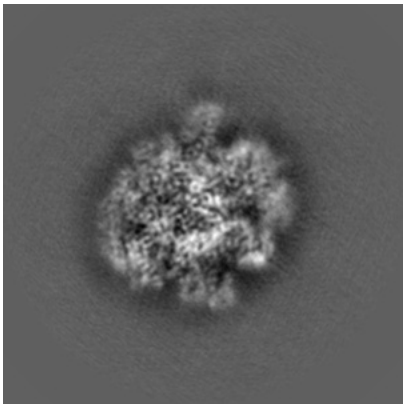


Z

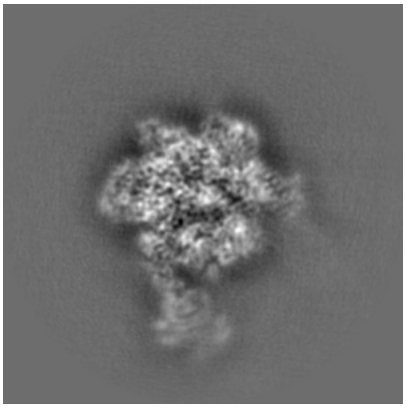
6.1.2 Raw map



X



Y

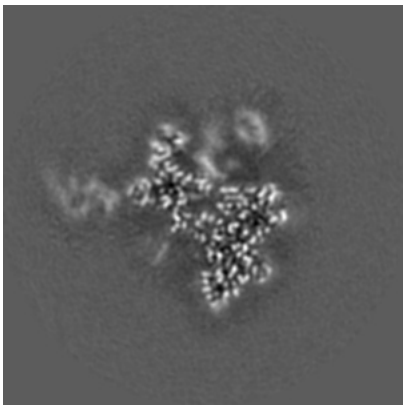


Z

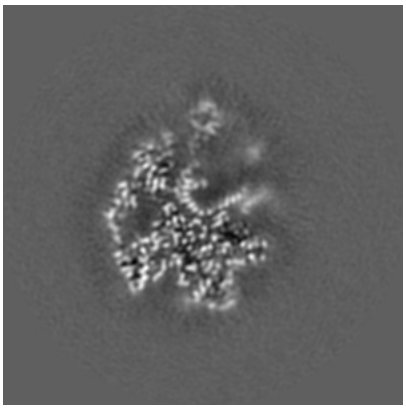
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

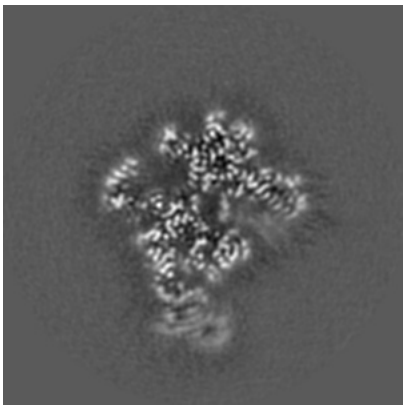
6.2.1 Primary map



X Index: 120

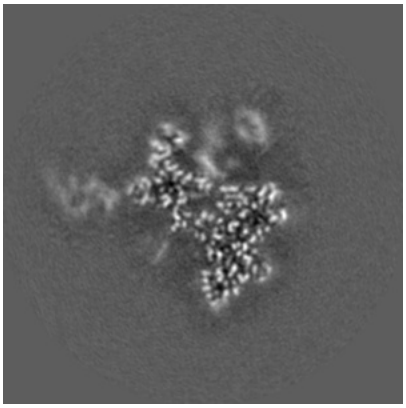


Y Index: 120

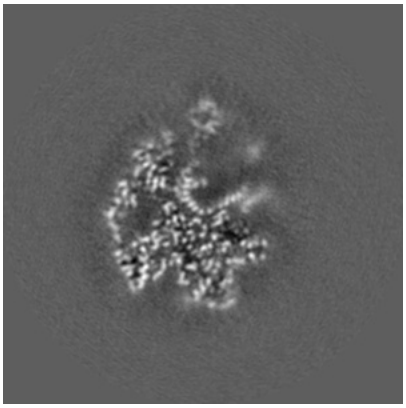


Z Index: 120

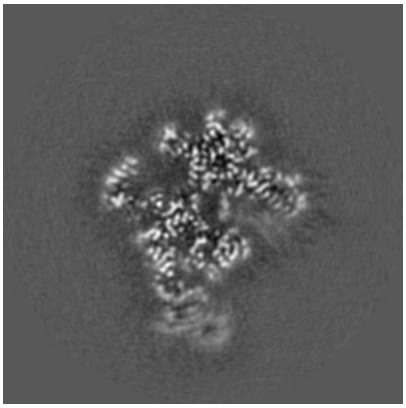
6.2.2 Raw map



X Index: 120



Y Index: 120

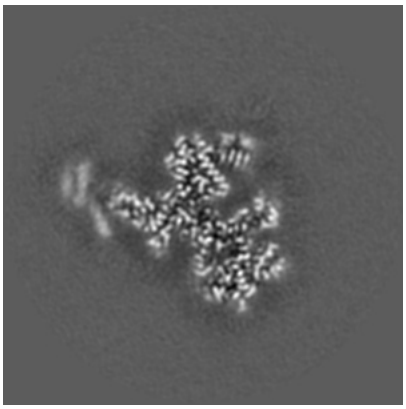


Z Index: 120

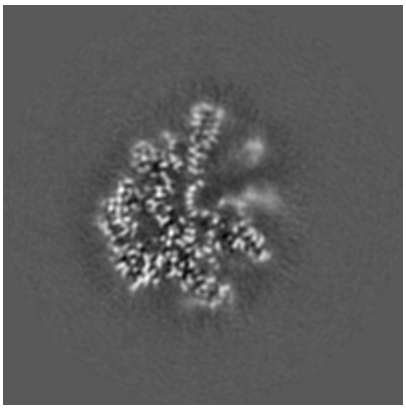
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

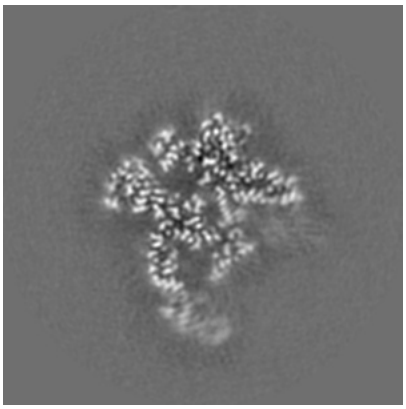
6.3.1 Primary map



X Index: 96

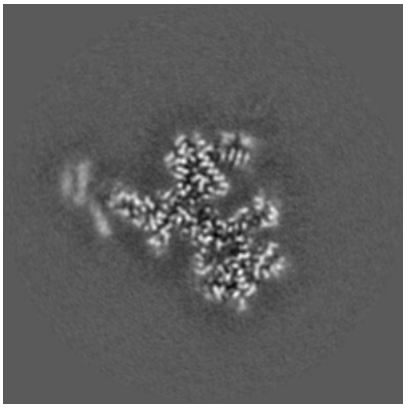


Y Index: 124

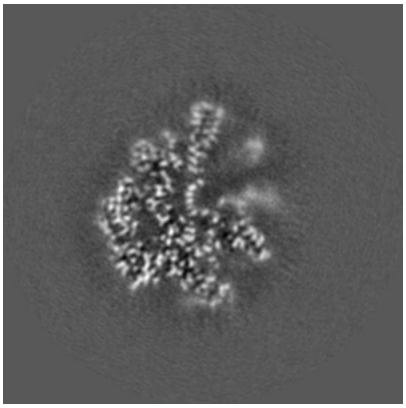


Z Index: 115

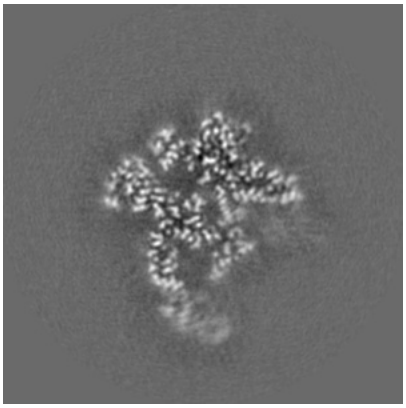
6.3.2 Raw map



X Index: 96



Y Index: 124

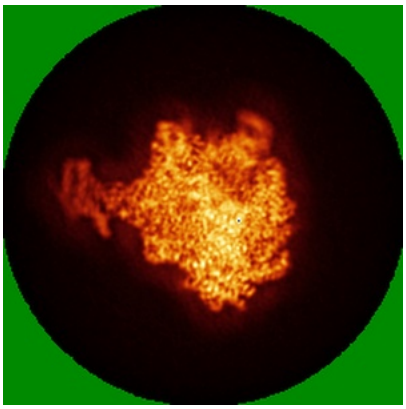


Z Index: 115

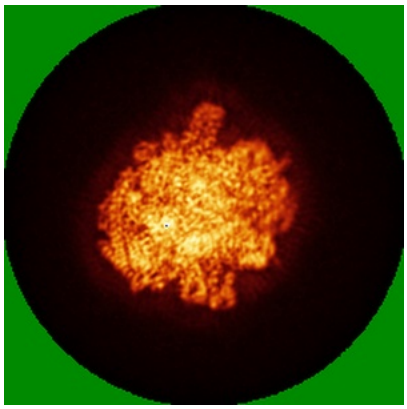
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

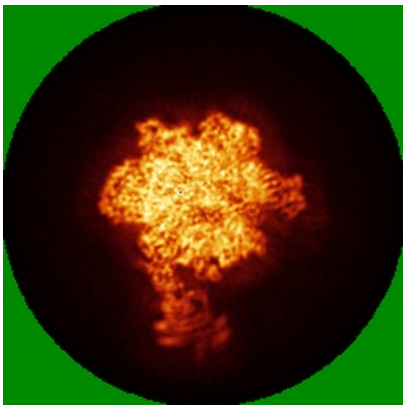
6.4.1 Primary map



X

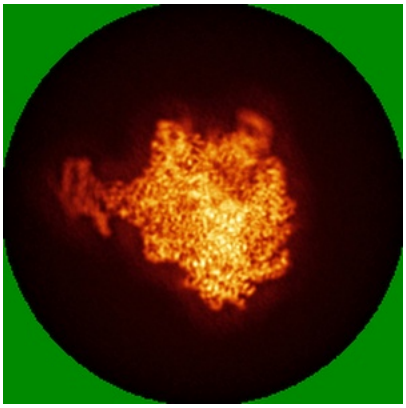


Y

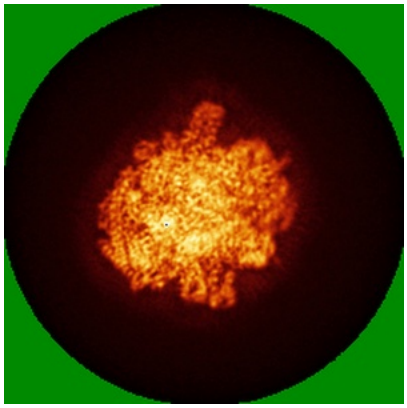


Z

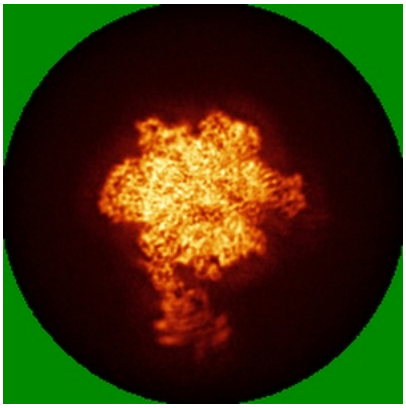
6.4.2 Raw map



X



Y

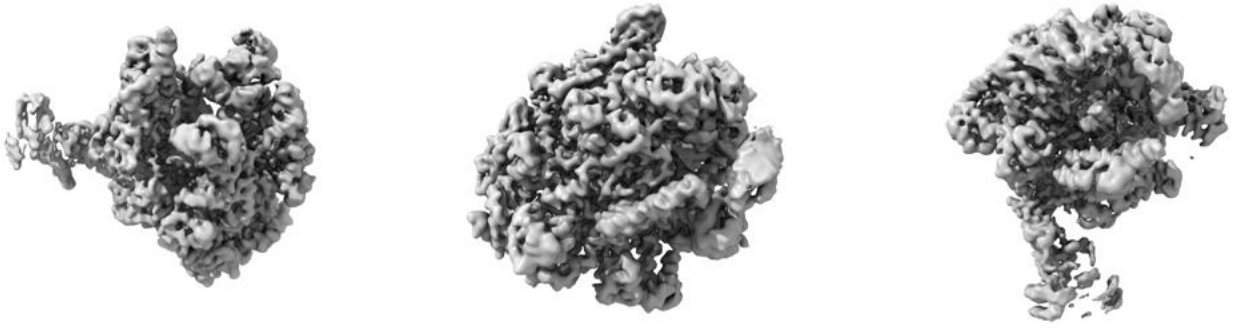


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

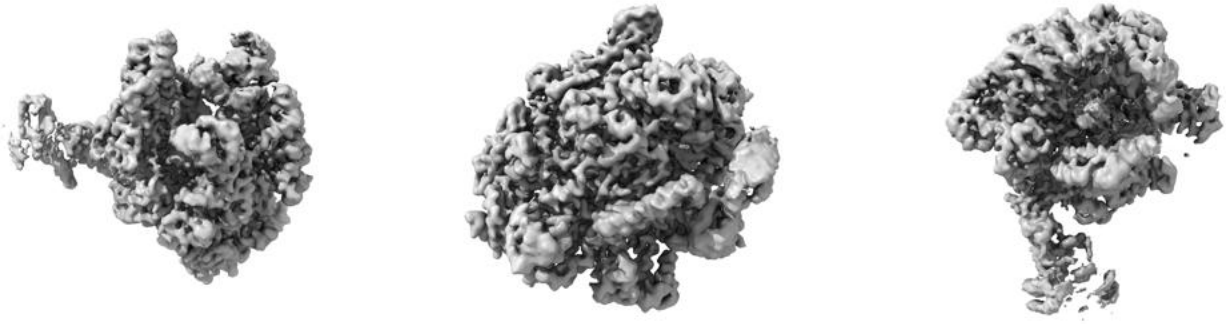
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

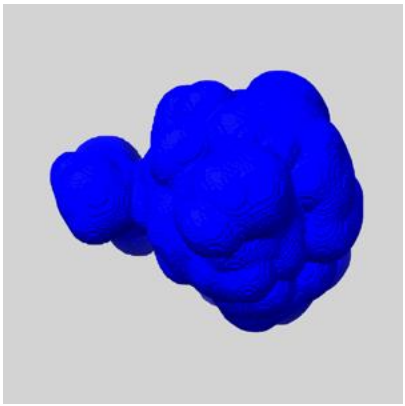
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

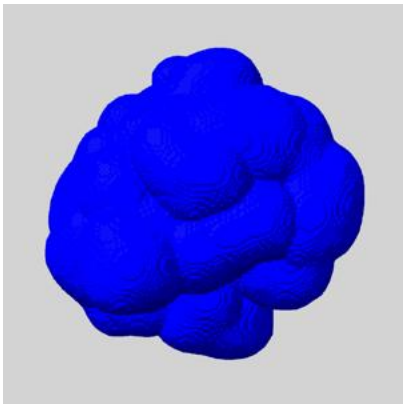
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

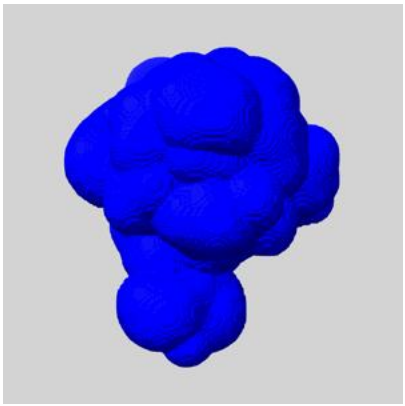
6.6.1 emd_16809_msk_1.map (i)



X



Y

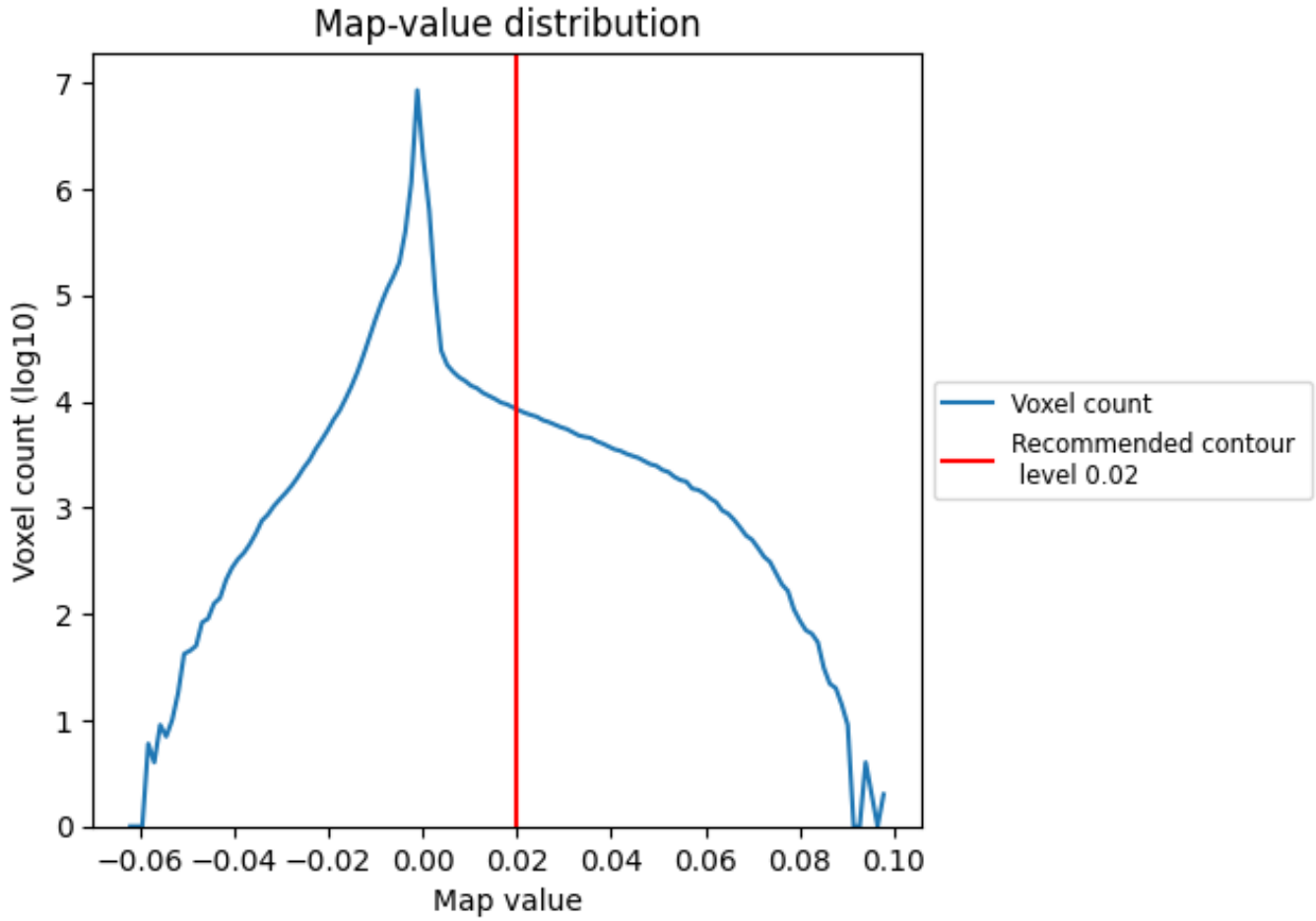


Z

7 Map analysis

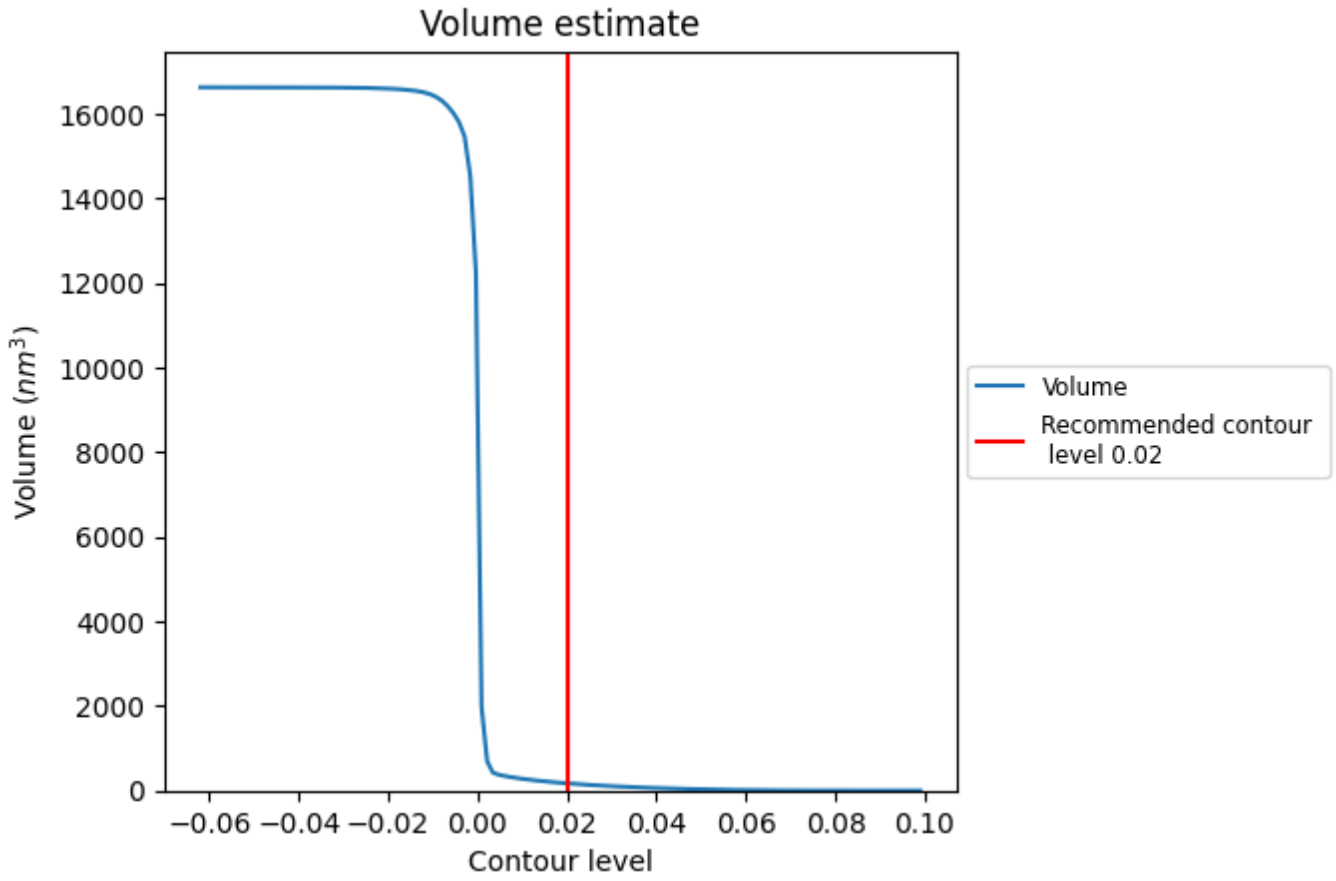
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

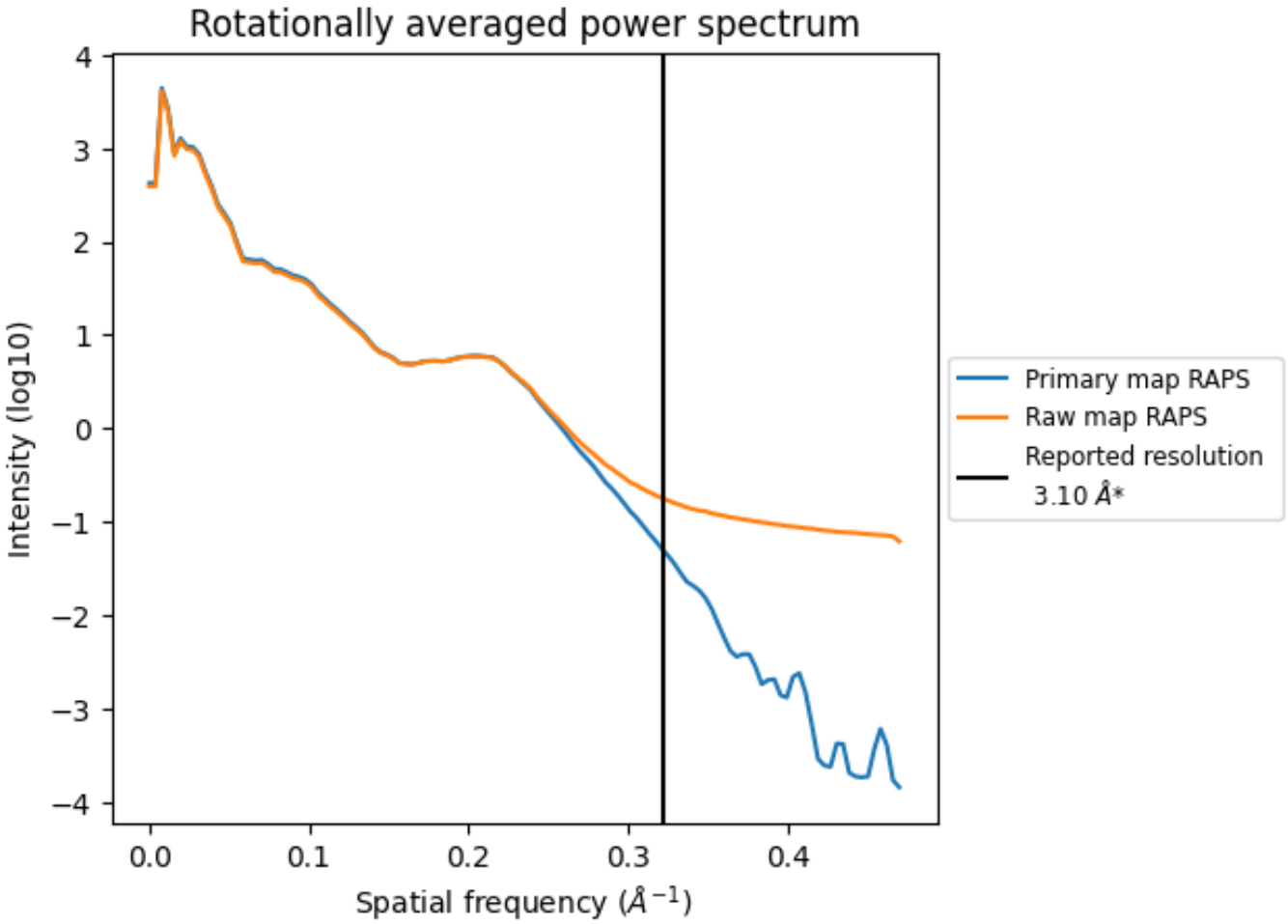
7.2 Volume estimate



The volume at the recommended contour level is 171 nm^3; this corresponds to an approximate mass of 154 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

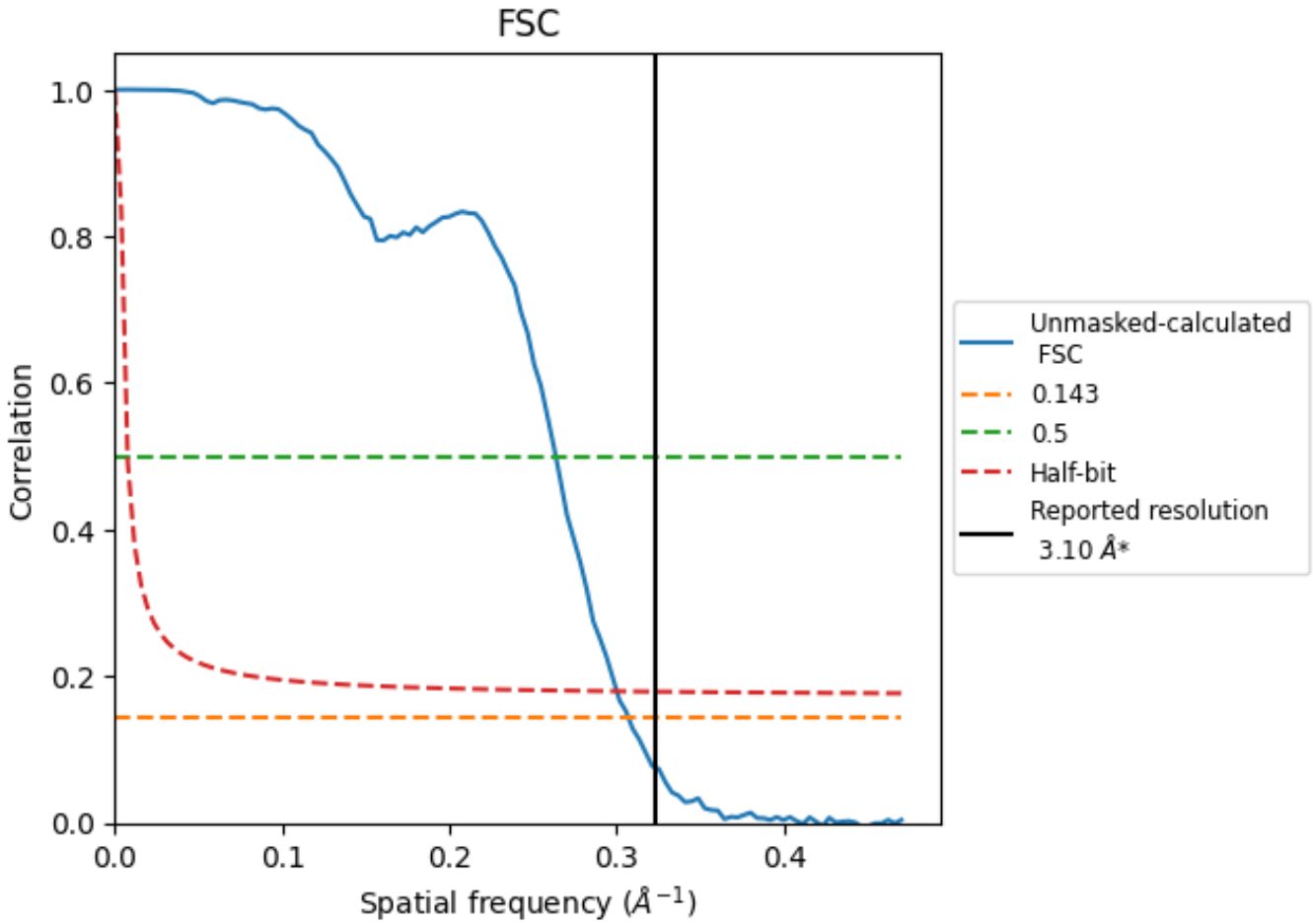


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

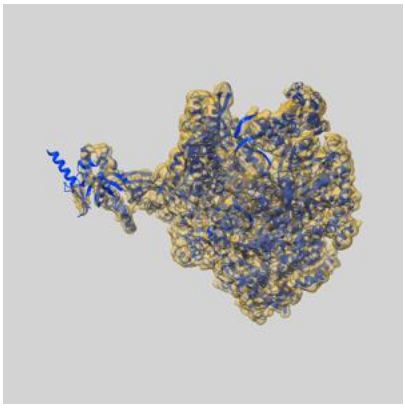
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.79	3.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

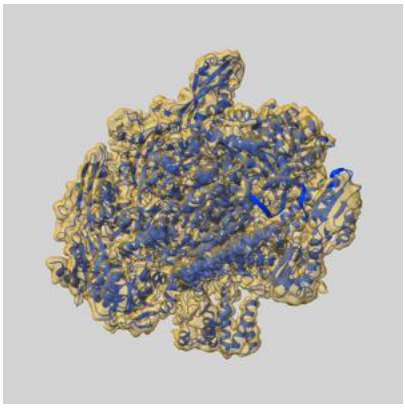
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16809 and PDB model 8CRO. Per-residue inclusion information can be found in section 3 on page 7.

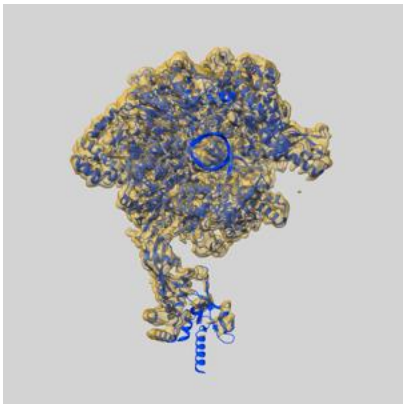
9.1 Map-model overlay



X



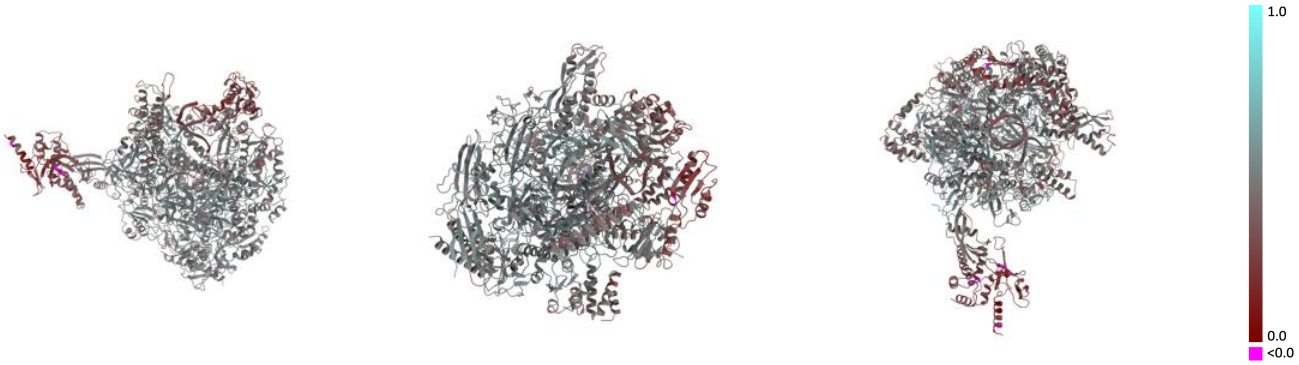
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

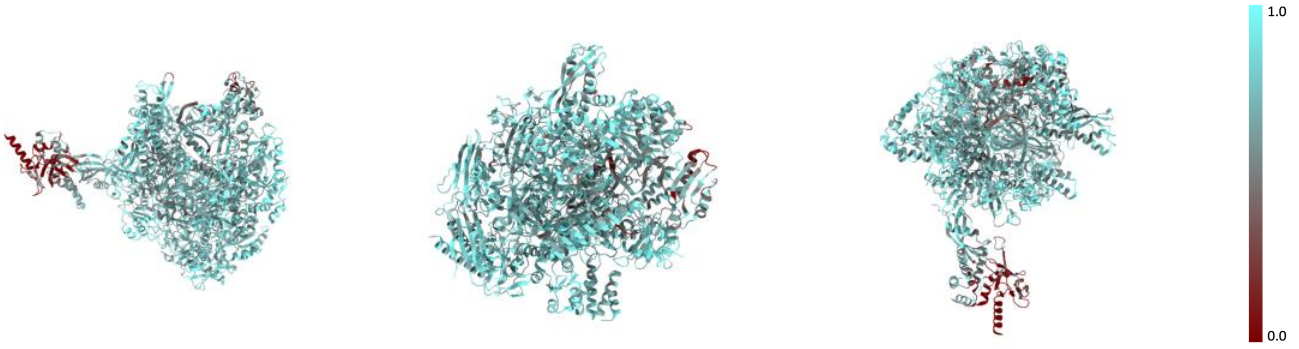
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

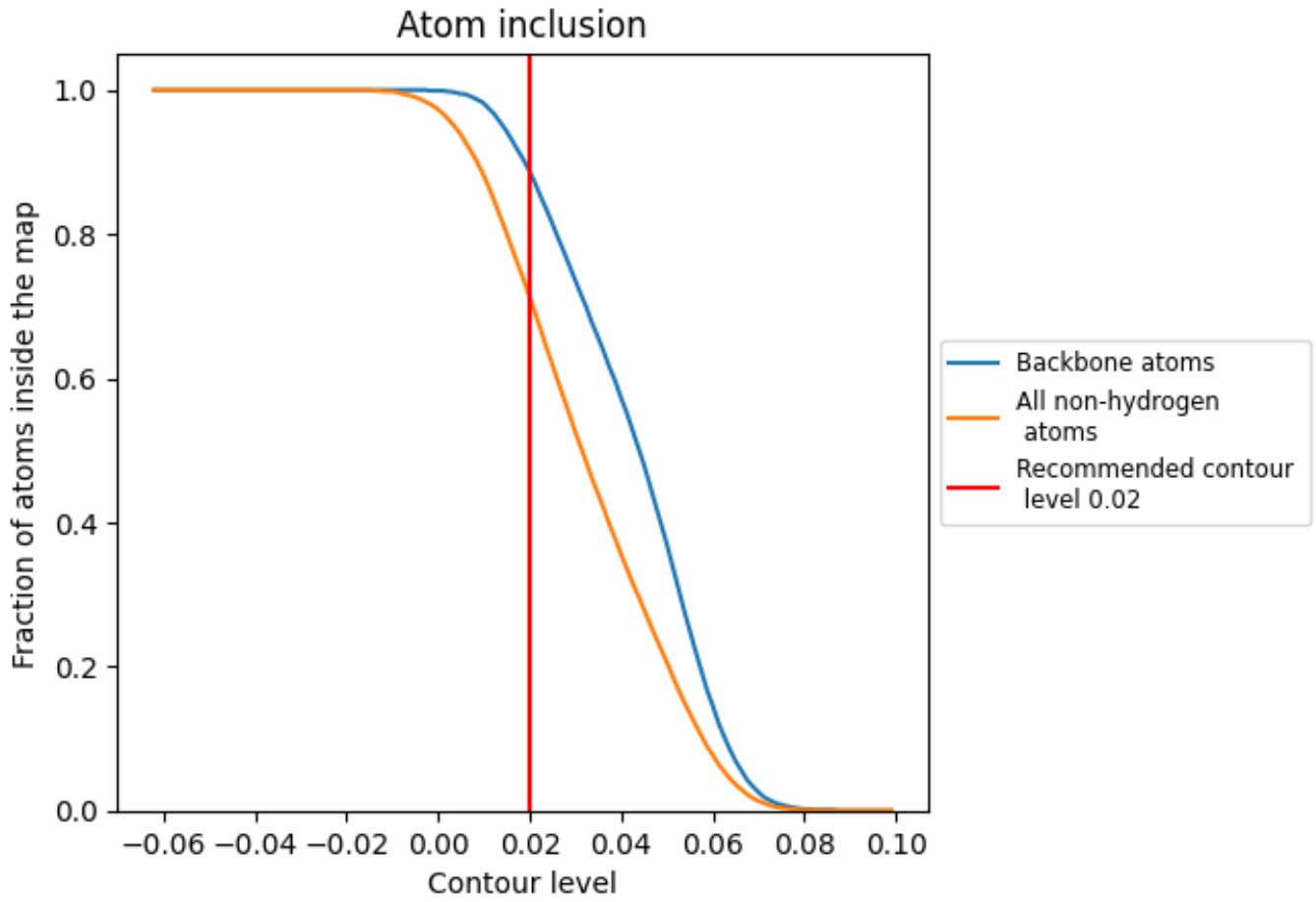
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.4620
A	0.7630	0.4850
B	0.7360	0.4850
C	0.6490	0.4120
D	0.7900	0.4960
E	0.3720	0.3240
F	0.5130	0.2940
H	0.8260	0.5010
K	0.8120	0.5060
L	0.7970	0.4950
N	0.8040	0.5140
P	0.7060	0.4660
X	0.7420	0.4430
Y	0.4770	0.3230
Z	0.8060	0.4870